

Joint Event

European Congress on

Chemistry and Applied Sciences

&

International Conference on

Catalysis and Chemical Engineering

March 20-21, 2023

Belstay Roma Aurelia, Rome, Italy



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Conference Programme

Conference Programme

Day 1: March 20, 2023

March 20-21, 2023, Belstay Roma Aurelia, Rome, Italy

Day 1, March 20, 2023

Meeting Hall: Parioli 1

8.30 - 9.00

Registrations

9.00 - 9.15

Introduction

Keynote Presentations

9.15 - 10.00

Stanislaw Dzwigaj, Sorbonne Université, France

Title: Application of Metal Single-Site Zeolite Catalysts in Heterogenous Catalysis

10.00 - 10.45

Sahn Nahm, Korea University, South Korea

Title: Growth of Crystalline NaNbO_3 Thin Film on $\text{Sr}_2\text{Nb}_3\text{O}_{10}$ Template at Low Temperatures for Piezoelectric Thin Film Energy Harvester

Group Photo: 10.45 - 11.00

Networking and Refreshments @ Bar: 11.00 - 11.20

Oral Presentations

Session Chair:

Stanislaw Dzwigaj, Sorbonne Université, France

Sessions: Catalysis for Chemical Synthesis | Chemical Engineering | Catalysis and Energy | Organocatalysis | Catalysis and Zeolites | Catalysis and Pyrolysis | Organometallics Chemistry | Catalysis in Nanotechnology | Catalysis and Applications | Biocatalysis and Biotransformations | Computational Catalysis | Surface and Colloidal Phenomenon | Photo catalysis and Electrochemistry | Enzymes and Biocatalysts | Fluid dynamics & its Phenomena | Catalysis for Renewable sources | Polymer for Science and Technology | Thermal Catalysis | Catalysis in Oil & Gas and Petrochemical Engineering | Environmental Catalysis | Catalytic Materials & Mechanisms | Enantioselective Catalysis | Industrial Catalysis | Simulation and Modeling in Catalysis

11.20 - 11.45

Višnja Vrdoljak, University of Zagreb, Croatia

Title: Geometrically Constrained Molybdenum (VI) Metallosupramolecular Architectures: Synthesis, Structure, and Properties

11.45 - 12.10

Jianli Hu, West Virginia University, USA

Title: Co-Processing of Biomass-Methane- CO_2 for Hydrogen Production

12.10 - 12.35

Gabriele Micheletti, University of Bologna, Italy

Title: Naphtoquinone Derivatives as Potential Anticancer Compounds

12.35 - 13.00

Suni Rodriguez, University of Basque Country, Spain

Title : Study of the Synergy between VGO and HDPE Pyrolysis Waxes in the Hydrocracking over NiW-Y Zeolites Catalysts

Lunch @ Seguimi: 13.00 - 14.00

14.00 - 14.25

Subhadip Ghosh, National Institute of Science Education and Research, India

Title: Perovskite Nanocrystals- Novel Material for Real Applications

14.25 - 14.50

Alexandra Jakab Nácsa, BorsodChem Zrt., Hungary

Title : Classification of Catalysts with MIRA21 Model in Heterogeneous Catalytic Hydrogenation of Aromatic Nitro Compounds

14.50 - 15.15

Su-Hwan Go, Korea University, South Korea

Title: Piezoelectric Properties of the [001]-Textured (Na, K)NbO₃-Based Lead-Free Piezoceramics and their Application to Piezoelectric Energy Harvesters

15.15- 15.40

Sudip Barman, NISER- Bhubaneswar, India

Title : Metal Nanostructures for Electrochemical Energy Conversion and Storage

15.40 - 16.05

Seokjune Chae, Korea University, South Korea

Title: Enhancement of Electromechanical Coupling Factor of the (Na, K)(Nb_{1-x}Sb_x)-SrZrO₃-(Bi, Ag)ZrO₃ Piezoceramics for Piezoelectric Energy Harvester

Networking and Refreshments @ Bar: 16.05 - 16.30

16.30 - 16.55

Alberto Ubaldini, ENEA, Italy

Title: Synthesis and Characterization of Borate Nanoparticles

16.55 - 17.20

Hamza Chanouri, Mohammed VI Polytechnic University, Morocco

Title: Integrated Valorisation of Phosphogypsum using pH Dependent Purification Process

17.20 - 17.45

Nurul Huda Abdul Wahab, Universiti Malaysia Terengganu, Malaysia

Title: Extended Study on Data Analysis For Investigating Chemical Profiles from MeOH Crude of Euphorbia Mili Flowers Applying GC-MS

17.45 - 18.10

Fawzi M. Elfghi, Libyan Petroleum Institute, Libya

Title: Combined Application of Response Surface Methodology (RSM) and Artificial Neural Network (ANN) based on Experimental Design (DOE) in Modeling and Optimization HDS Activity

18.10 - 18.35

Anasse Sraidi, Mohammed VI Polytechnic University, Morocco

Title: Recovery of Rare Earth Elements from Phosphoric Acid using Ion Exchange Resin

Day Concludes

Day 2: March 21, 2023

Meeting Hall: Parioli 1

Keynote Presentation

10.00 - 10.45

Blaz Likozar, Kemijski Inštitute, Slovenia

Title: Hydrogen, Ammonia, CCU and beyond – Electrification of Industrial Unit Operations

Oral Presentations

Session Chair:

Višnja Vrdoljak, University of Zagreb, Croatia

Sessions: Organic Chemistry | Inorganic Chemistry | Food Science | Forensic Science | Agricultural Sciences | Computer Sciences | Renewable Energy | Medicinal Chemistry | Physical Chemistry | Analytical Chemistry | Material Science | Nanomaterials | Chemical Engineering | Green Chemistry | Polymer Chemistry | Industrial Chemistry | Natural Products and Peptide Chemistry | Marine & Petro Chemistry | Catalysis | Applied Chemistry | Metallurgy | Geochemistry | Food Chemistry

10.45 - 11.10

Belkacem Merzouk, University of M'sila, Algeria

Title: Evaluation of the Efficiency of Coagulation-Flocculation Process for Treatment of Textile Wastewater using Anatural Flocculant - Cactus *Opuntia Ficus Indica*

11.10 - 11.35

Tofik Nagiev, Azerbaijan National Academy of Sciences, Azerbaijan

Title : New Approaches to Simulation of Enzymatic Reactions: Mimetic Catalysis

Networking and Refreshments @ Bar: 11.35 - 12.00

12.00 - 12.25

Taghreed M. A. Jazzazi, Yarmouk University, Jordan

Title: New Schiff Base Ligands and their Corresponding Zinc Complexes. Synthesis, Characterization and Computational Study

12.25 - 12.50

Madhumita Dandopath Patra, Acharya Prafulla Chandra College, India

Title: Understanding Protein-Sugar Interactions Using Molecular Modeling Techniques

Lunch @ Seguimi: 12.50 - 13.50

Poster Presentations (13.50 - 16.00)

PP001

E A Jaseer, KFUPM University, Saudi Arabia

Title : Solvent-Free Iridium-Catalyzed Synthesis of Silyl Carbamates from the Reaction of Amines with Carbon Dioxide and Hydrosilanes

PP002

Ujuagu Akunna Frances, Tohoku University, Japan

Title: Designing a Light-Up Peptide Probe as an FID Assay Indicator for RNPs

PP003

Niladri Maity, KFUPM University, Saudi Arabia

Title : Silica-Supported Monoalkylated Tungsten Dioxo Complex Exhibits Catalytic Olefin Metathesis Reaction

PP004

Slavica Marinović, INA – Industrija nafte PLC, Croatia

Title: Diamondoid Hydrocarbons as Maturity Indicators for High Maturity Crude Oils and Condensates

PP005

Nestor Garcia Villalta, KFUPM University, Saudi Arabia

Title : Aryl-Di(Pyridil) Pyrrole Group IV Complexes as Catalyst in Ethylene Polymerization

PP006

Kai Dollevoet, Charles River Laboratories, Netherlands

Title: The Applicability of Rotational Viscosity within the Scope of Safety Assessment of Agrochemicals

PP007

Sathiyamoorthy Murugesan, KFUPM University, Saudi Arabia

Title : Surface Modified Mesoporous Materials for Petrochemical Refining Processes

PP008

Alessio Pelucelli, Università di Sassari, Italy

Title: Biological Effects of Human Exposure to Environmental Cadmium

PP009

Iwan Iwanov, University of Chemical Technology and Metallurgy, Bulgaria

Title: Catalytic Transformation of Ribose to Furfural in Presence of HCl

PP010

Arancha Saiz Valderrama, University of Basque Country, Spain

Title: LTA Packed Bed Membrane Reactors for DME Synthesis from CO₂ and CO₂/CO_x Mixtures: Crystallization of the Membrane

PP011

Krzysztof Moraczewski, Kazimierz Wielki University, Poland

Title: The Use of After Printing Process Waste as a Filler for Polymer Materials

PP012

Mory Traore, University of Science and Technology Beijing, China

Title: Enhanced Oil Removal and Reduction of Activated Sludge by Ozonation Efficiency of a New Microbubble Generator

PP013

Mirna Biondić, INA – Industrija nafte PLC, Croatia

Title: Paraffin Wax in Petroleum Industry: A Review on Formation, Experimentation, Prevention, and Removal Techniques

PP014

Dan Gowland, University of Edinburgh, UK

Title : LED-Driven Photocatalytic Oxidation Technology for Water Purification

PP015

Abdelhak Mesbah, Djillali LIABES University (UDL), Algeria

Title: Retention Study of an Organic Persistent Molecule by Surfactant Clay Composite (Clay-C18Tab)

Networking and Refreshments @ Bar: 16.00 - 16.30

16.30 - 16.55

Alberto Ubaldini, ENEA, Italy

Title: A Characterization Of Na₂Mo₄, Na₂Wo₄ and their Solid Solution

16.55 - 17.20

Fabián Espitia-Almeida, Universidad Simón Bolívar, Colombia

Title: Synthesis and Antibacterial Photodynamic Activity of the New Photosensitizer 5,10,15,20-Tetrakis(4-Ethylphenyl)Porphyrin

Video Presentation

VP001

Tatyana Ryazanova, Samara State Medical University, Russia

Title: Application of Ethylcellulose-based Sorbent for Solid-Phase Extraction for Quantitative Determination of Benzoic acid in Medicinal Products

Day 2 Concludes followed by Panel Discussion - Awards & Closing Ceremony

Conference Programme

Virtual Programme

March 20-21, 2023, Virtual Program

Day 1 March 20, 2023 GMT (London Time: 10.00 - 16.25)

Keynote Presentation

10.00 - 10.30

Muhammad Atiqullah, KFUPM University, Saudi Arabia

Title: Making Ethylene-Alpha Olefin Elastomer: Investigation of Liquid Phase Catalyst Active Center Residential Environment and New Results

Oral Presentations

10.30 - 10.55

Ravichandran, Lovely Professional University, India

Title: Environmental Friendly Plastic Waste Management

10.55 - 11.20

Prerna Sharma, Guru Gobind Singh College of Pharmacy, India

Title: The Pharmacological Activity of Tulsi (*Ocimum sanctum*)

11.20 - 11.45

Basharat Hussain, Chung Yuan Christian University, Taiwan

Title: Free-Metal Catalyst of Layered Double Hydroxide/PET polymer for Efficient Thermomechanical and Barriers

11.45 - 12.10

Tadios Tesfaye Mamo, Taiwan University, Taiwan

Title: Waste-Based Nanocatalysts for Biofuel (Biodiesel) Production

12.10 - 12.35

Meena Nemiwal, Malaviya National Institute of Technology, India

Title: Chloroaluminate $[\text{HN}_{222}][\text{Al}_2\text{Cl}_7]$ Ionic Liquid Immobilized on the Copper (II) Oxide Nanoparticles $\{\text{CuO}[\text{HN}_{222}][\text{Al}_2\text{Cl}_7]\}$ Used in Case Study of Chan-Evans-Lam Coupling approach

12.35 - 13.00

Daria Nekhorosheva, National Research University Higher School of Economics, Russia

Title: Potential of Green Chemistry in Smart Cities' Renewable Energy

Lunch (13.00 - 13.30)

13.30 - 13.55

Eleonara Butenko, Azov Sea State Technical University, Ukraine

Title: Retroaldol Cleavage over Layer Double Hydroxides: Effect of Metal Components on Selectivity and Activity

13.55 - 14.20

Jyoti Rajput, Lovely Professional University, India

Title : Emerging Technology of laser beat wave electron acceleration in vacuum

14.20 - 14.45

Faryal Idrees, The University of the Punjab, Pakistan

Title: Synthesis and Characterizations of MoS₂/Wo₃ Heterostructures for Efficient Photocatalytic Efficiency

14.45 - 15.10

Mexis D, National And Kapodistrian University Of Athens, Greece

Title: Effect of A 6 Week Preseason Training Program on Salivary Biomarkers in Elite Basketball Athletes

15.10 - 15.35

Isaac Yissa Aaron, University of Ilorin, Nigeria

Title: Metal-Organic Coordination Compounds of Manganese(II) Containing Terephthalate, Bipyridine, and Terpyridine Ligands: Syntheses, Crystal Structures and Catalytic Oxidation Properties

15.35 - 16.00

Haibo Ge, Texas Tech University, USA

Title: Distal Functionalization via Transition Metal Catalysis

16.00 - 16.25

Orlando Elguera Ysnaga, Universidade de São Paulo, Brazil

Title: Review of Research Topics for Scaling-up of Sonochemical Reactors (Sono-Reactors)

Day 1 Concludes

Day 2 March 21, 2023 GMT (London Time: 10.00 - 13.45)

Keynote Presentations

10.00 - 10.30

Siquan Feng, Chinese Academy of Science, China

Title: Sulfur-Poisoning on Rh Nanoparticle but Sulfur-Promotion on Single-Rh₁-site for Carbonylation

10.30 - 11.00

Tokeer Ahmad, Jamia Millia Islamia, India

Title: Nanocatalysis for Hydrogen Generation

Oral Presentations

11.00 - 11.25

Felix Panis, University Of Vienna, Austria

Title: Tyrosinases in Wetlands: Global Contributors to Climate Change!

11.25 - 11.50

Rajesh Kumar, R.D.S. College (B.R.A. Bihar University), India

Title: Biocatalyst Mediated Synthesis of Modified Nucleosides

11.50 - 12.15

Muhammad Umer Sohail, Institute of Space Technology, Pakistan

Title: Effect of Secondary Combustion on Thrust Regulation of Gas Generator Cycle Rocket Engine

12.15 - 12.40

Labode Stevenson Naitchede, Institute for Basic Sciences, Technology, and Innovation, Kenya

Title: Transcript Expression Level Analysis of Phytoene Synthase and Phytoene Desaturase Associated with β -Carotene Content and Genetic Transformability in Bitter Melon

12.40 - 13.05

Prem Kumar Jaiswal, Retired Director Of Labs, India

Title: National Food Control System in India

13.05 - 13.30

Sandip Kumar Lahiri, National Institute of Technology, India

Title: Artificial Intelligence Based Modelling and Optimization of Catalyst in Real Industrial Plant to Simultaneously Enhance Profit and Reduce Negative Environmental Impact

13.30 - 13.55

Viacheslav Artyushenko, Art Photonics GmbH, Germany

Title: Chemical Process-Control in line with 4 Methods of Fiber Spectroscopy

13.55 - 14.20

Eleonora Aneggi, University of Udine, Italy

Title: Heterogeneous Fenton-Like Process over Steel Scale waste for the Treatment of Landfill Leachate

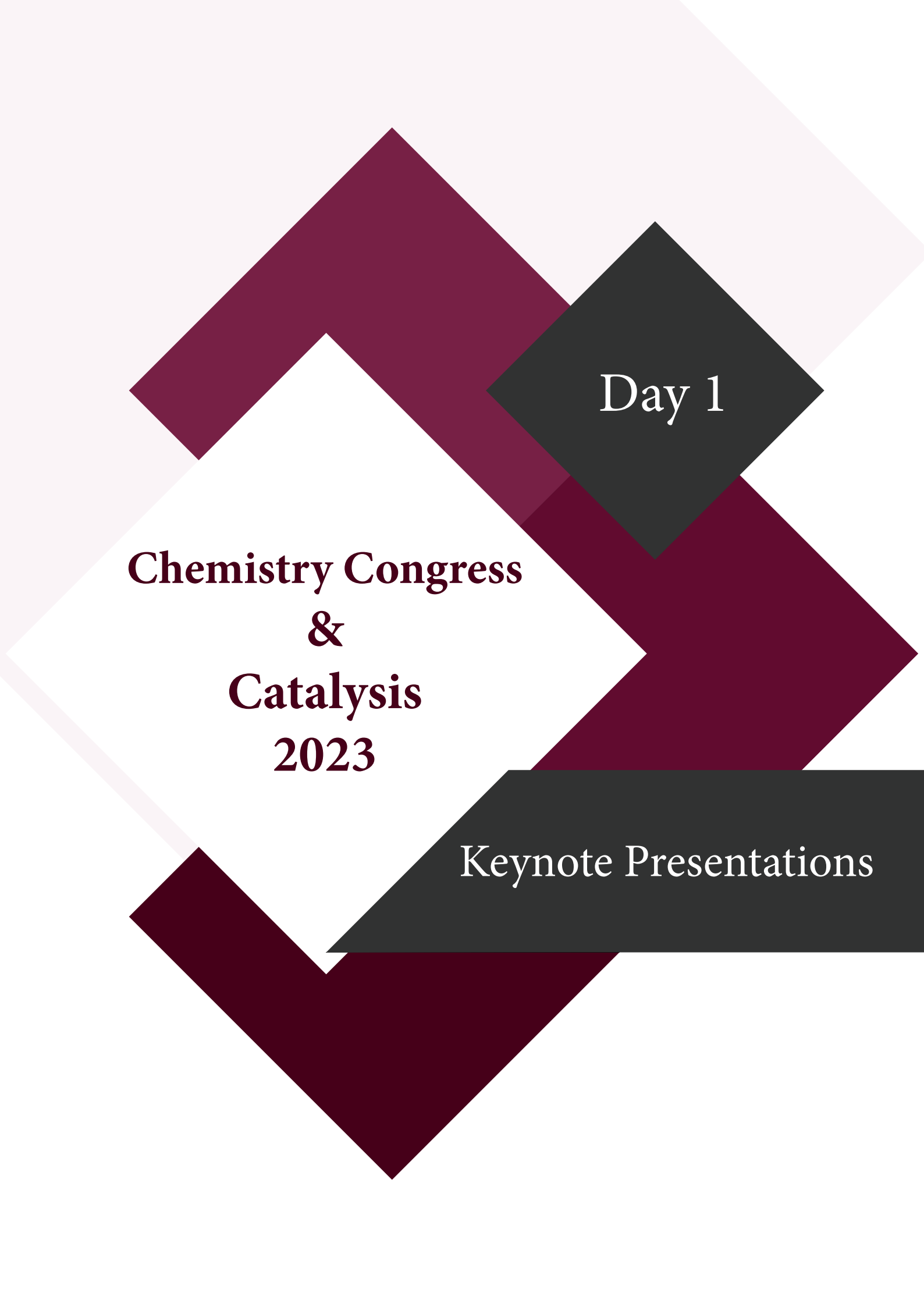
Poster Presentation

14.20 - 14.35

Ali Zeinodiny, Tarbiat Modares University, Iran

Title: Investigating the Performance of Spinel Materials MgX_2O_4 ($x=Mn, Ni, Co$) as Potential Cathodes in Magnesium-Ion Batteries

Day 2 Concludes Followed by Vote of Thanks



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Day 1

Keynote Presentations

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APPLICATION OF METAL SINGLE-SITE ZEOLITE CATALYSTS IN HETEROGENEOUS CATALYSIS



Stanislaw Dzwigaj

Sorbonne Université, France

Abstract:

The metal ions well dispersed at zeolite framework are considered to be active sites of catalytic processes. Therefore, the incorporation of these metals into zeolites as isolated tetrahedral sites appears to be the important task. We have earlier shown that the incorporation of transition metal ions into vacant T-atom sites of framework zeolite is strongly favored when, in the first step, zeolite is dealuminated by treatment with nitric acid solution and then, in the second step, the incorporation of transition metal ions results in the reaction between the cationic metal species of the precursor solution and the SiO-H groups of vacant T-atom sites created by dealumination of zeolite. During my keynote talk the design of single-site zeolite catalysts with transition metal will be described and characterized by different physical techniques both at the macroscopic (XRD, BET, TPR, TEM) and molecular level (FT-IR, NMR, DR UV-Vis, XPS, EPR, XAFS). The application of metal single-site zeolite catalysts in environmental catalysis will be discussed. This two-step postsynthesis method applied in this work allowed obtaining metal single-site zeolite catalysts active in different catalytic processes such as oxidative dehydrogenation of propane into propene, selective catalytic reduction of NO_x to N_2 , production of 1,3-butadiene or hydrogen from renewable sources, including ethanol obtained from biomass. Their catalytic activity strongly depended on the speciation and amount of metal incorporated into zeolite structure as well as their acidity.

Biography

Stanislaw Dzwigaj received his PhD degree in 1982 in Jerzy Haber Institute of Catalysis and Surface Chemistry, Krakow (Poland). After two years of postdoctoral stay at the Laboratoire de Réactivité de Surface Université P. et M. Curie (Paris) he obtained in 1990 a position of contracted researcher in the same Laboratory devoted to surface reactivity in relation to catalysis phenomena. Then, in 2008 he obtained permanent position in CNRS as a researcher. On February 19, 2014 for outstanding scientific achievements, he received the title of professor. His published work includes more than 170 papers published in reputable international journals.

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GROWTH OF CRYSTALLINE NaNbO_3 THIN FILM ON $\text{Sr}_2\text{Nb}_3\text{O}_{10}$ TEMPLATE AT LOW TEMPERATURES FOR PIEZOELECTRIC THIN FILM ENERGY HARVESTER



Sahn Nahm

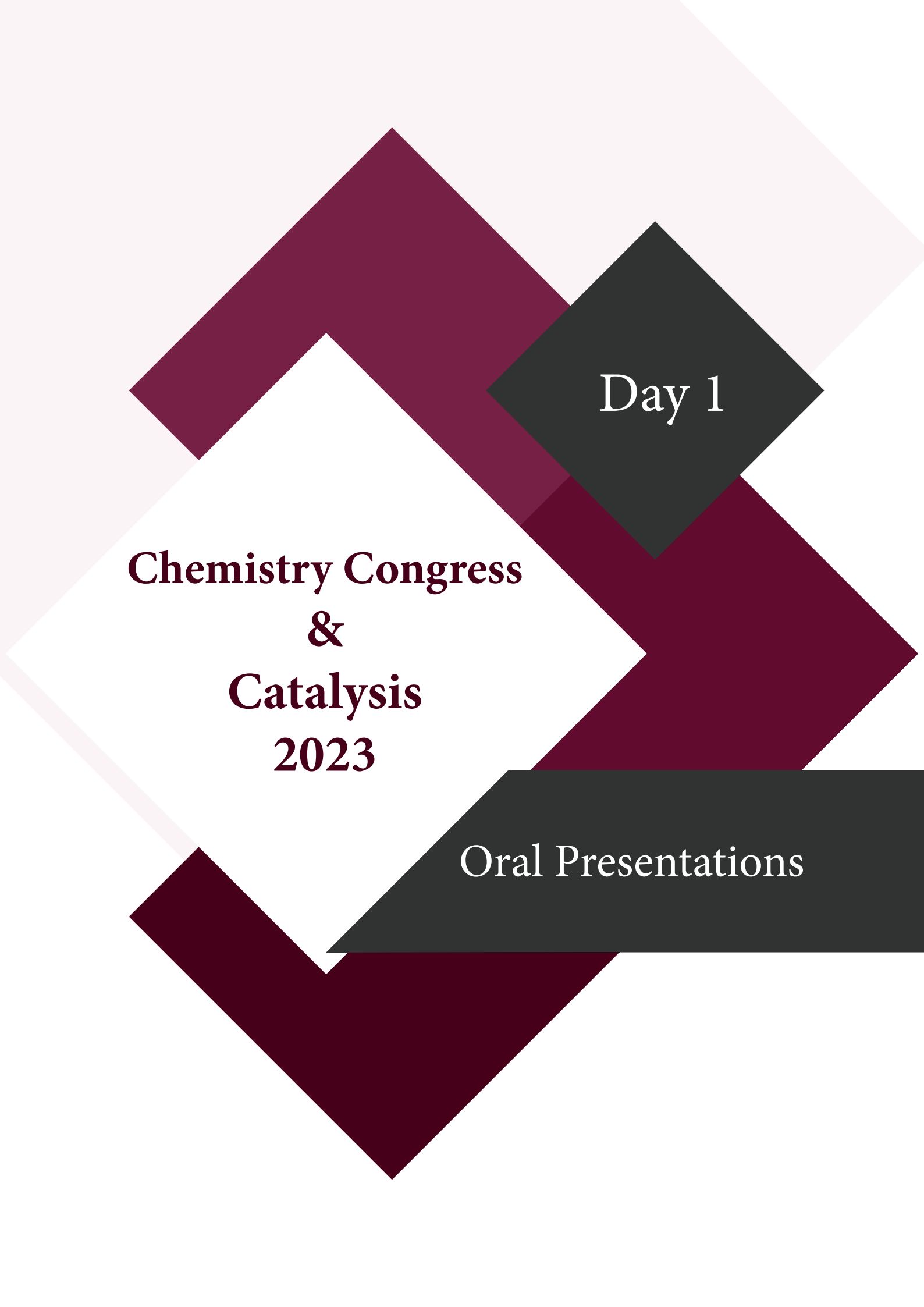
Korea University, South Korea

Abstract:

A $\text{Sr}_2\text{Nb}_3\text{O}_{10}$ (SNO) monolayer deposited on Pt/SiO₂/Si (PSS) was employed as the template for the growth of crystalline NaNbO_3 (NN) thin films at low temperatures. The [001]-oriented crystalline NN film was effectively grown on SNO/PSS at 250°C. This NN film showed a small ϵ_r of 115, along with good insulating properties with a low leakage-current density (4.5×10^{-6} A/cm² at 0.3 MV/cm). This NN film displayed a large d_{33} of 123 pC/N, which is the largest d_{33} value for NN films to date. Moreover, it shows a very large $d_{33} \times g_{33}$ (14.8×10^{-12} m²/N), which is the figure of merit for the power of piezoelectric energy harvester (PEH). The NN film grown on SNO/Ni at 250°C for the fabrication of thin film PEH also demonstrated outstanding dielectric and piezoelectric characteristics. The NN thin film PEH exhibited a high power density ($2.1 \mu\text{W}/\text{mm}^3$), indicating the [001]-oriented NN film grown on the SNO seed layer is a good candidate for thin film PEH. Moreover, this NN film can be deposited on a polymer substrate and utilized as a future flexible device owing to its very low growth temperature and good physical properties.

Biography

Sahn Nahm received the Ph.D. degree from University of Maryland, College Park, USA in 1990. And he was a Postdoctoral Research Associate in University of Maryland between 1991 and 1992. He was a Senior Researcher in the Electronic Telecommunication Research Institute in Korea from 1992 to 1995 and moved to Keimyung University, Dae-gu, Korea, in 1995. Since February 1996, he is a faculty of the Department of Materials Science and Engineering, Korea University, Seoul, Korea where he is a Professor and the Head of the Electro-Ceramics Laboratory. He is a President of Korean Ceramics Society in 2022. His research fields are the dielectric thin films, piezoelectric ceramics and ReRAM.



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2023**

Day 1

Oral Presentations

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GEOMETRICALLY CONSTRAINED MOLYBDENUM(VI) METALLOSUPRAMOLECULAR ARCHITECTURES: SYNTHESIS, STRUCTURE, AND PROPERTIES

Višnja Vrdoljak

University of Zagreb, Croatia

Abstract:

Supramolecular architectures based on coordination compounds consisting of metal centres bridged by organic ligands are continuing to be an interesting area of research. Such structures exhibit a wide variety of properties and therefore represent attractive materials in connection with numerous possible applications. On the other hand, the reports on Mo(VI) metallosupramolecular compounds are relatively rare. The lack of examples is not surprising, as these compounds are difficult to synthesize. Namely, the MoO_2^{2+} core tends to polymerize through the $\text{Mo}=\text{O} \cdots \text{Mo}$ interaction.

Our research refers to the synthesis and characterization of cyclic $[\text{MoO}_2(\text{L})]_n$ complexes with polydentate aroylhydrazone ligands expected to exhibit superior catalytic activity. In this work, metallosupramolecular compounds were generated by conventional synthesis as well as by vapor and thermally induced solid-state structural transformations utilizing coordination-driven self-assembly of MoO_2^{2+} core and nicotinylhydrazonate or aminobenzoylhydrazonate ligands. The chemometric analysis using principal component analysis was applied to provide an insight into the reaction profile of the vapor-induced transformations. All compounds were characterized by the use of NMR spectroscopy and X-ray crystallography. The X-ray diffraction analysis revealed that the ligand was coordinated in the dianionic form to the *cis*- $\{\text{MoO}_2\}^{2+}$ core via the *ONO* donor atoms. The remaining sixth coordination site was occupied by the nitrogen atom N' of the aminobenzoyl or nicotinoyl moiety of the neighbouring molecule.

The potential of dinuclear or tetranuclear assemblies depends on their geometrically constrained nature and $\text{Mo}-\text{N}'$ bond distances. The use of the hemilabile ligands in small-sized cyclic Mo(VI) complexes offered easy access to highly reactive pentacoordinated species and, therefore, exquisite catalytic activity.

Biography

Višnja Vrdoljak received her Ph.D degree in Inorganic chemistry in 1996 from the Faculty of Science, University of Zagreb. Following a post-doctoral fellowship at the University of Trieste, Italy, she joined the Faculty of Science at the University of Zagreb. In 2015 she was appointed to the position of professor at the Department of Chemistry. Her current research interests are focused on the development of hybrid organic-inorganic polyoxometalate-based materials, metallosupramolecular architectures, and mononuclear complexes of molybdenum, vanadium, and tungsten for applications in catalysis. Her interests include the design, synthesis, and characterization of novel inorganic-organic hybrid materials intended for exhibiting a given property. Her interests also include studying the structure/property correlations.

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CO-PROCESSING OF BIOMASS-METHANE-CO₂ FOR HYDROGEN PRODUCTION

Jianli Hu

West Virginia University, USA

Abstract:

Transition from fossil fuels to renewable technologies is extremely challenging as renewable energy sources like solar, wind, and biomass are highly unreliable, subject to variation in geography and local climatic conditions. Transition from fossil hydrogen to renewable hydrogen is bridged by the unique 'natural gas – biomass co-processing'. At WVU, hydrogen rich syngas production through renewable hardwood biomass gasification was obtained through synergistic natural gas – biomass co-processing. About 5% methane co-processed with biomass at 850°C on Fe-Mo/CNF catalyst produces H₂:CO ratio of 6 with a very low CO₂ concentration of < 5% in the syngas. About 60 to 80% hydrogen was obtained in the product gas on the Fe-Mo/CNF, Ni-Mo/CNF, and Mo-Pd/CNF catalysts. Synergistic methane activated biomass gasification could be a promising technology for hydrogen rich syngas production as it requires very low concentrations of methane which could be obtained from flare gas. Flare gas is natural gas flared during commissioning of new wells or maintenance of existing wells in shale gas field. On-site utilization of flare gas with biomass could greatly curb CO₂ emission while producing hydrogen rich syngas. CO₂ utilization in the methane activated biomass gasification was studied by adding 1% CO₂ to the gas feed. CO₂ and CH₄ activation at high temperature was performed on Fe, Ni, and Pd active sites while Mo active sites are responsible for deoxygenation of oxygen rich biomass. In-situ conversion of raw biomass co-processed with 5% methane produces H₂-rich syngas on the carbon nanofiber supported catalyst. CNF support is also obtained from the biomass feedstock by impregnation with metals and pyrolysis at 700°C. This process is 95% renewable with net reduction in CO₂ emissions by recycling of CO₂. Detailed mechanistic investigation through molecular simulations helped ascertain the unique reaction pathway occurring on dual active sites on a transition metal doped β-Mo₂C-CNF catalyst. Application of renewable technologies is on the rise especially in power generation but is still far from being a mainstream source of hydrogen and power.

Biography

Jianli Hu is a Chair Professor and the Director of Shale Gas Center at West Virginia University. He leads an interdisciplinary team carrying out cutting edge research in natural gas conversion and renewable energy utilization. He has demonstrated strong leadership in partnering with U.S. national laboratories and industrial companies. His research interests span across the fields of reaction engineering, surface chemistry, plasma and microwave-enhanced catalytic reactions. Before joining WVU, Dr. Hu led innovation efforts at Koch Industries, Pacific Northwest National Laboratory and BP Oil. He has been granted 38 U.S. patents and published over 100 peer-reviewed journal articles and 200 conference papers.

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NAPHTHOQUINONE DERIVATIVES AS POTENTIAL ANTICANCER COMPOUNDS

Gabriele Micheletti

University of Bologna, Italy

Abstract:

In recent years, quinonic compounds are experiencing considerable interest due to their both anticancer and pro- or anti-oxidant capacity. A series of naturally occurring naphthoquinones was reacted, in mild conditions, with *N-acetyl-L-cysteine* and the related thia-Michael-like adducts were obtained. After the tuning of the reaction conditions, the reaction products were isolated as almost pure from the complex reaction mixture *via* simple filtration and were fully characterized. In the case of 1,4-naphthoquinone, by increasing the reaction temperature, a diadduct was obtained in high yield. Once obtained and isolated the novel derivatives, their biological activity was evaluated on a panel of human cancer cell lines [cervical carcinoma (HeLa), neuroblastoma (SH-SY5Y), and osteosarcoma (Saos-2 and U-2 OS)] and in normal.

dermal fibroblasts (HDFa) to evaluate their selective activity. The induction of reactive oxygen species (ROS) by the novel 1,4-naphthoquinone derivatives was also evaluated. The MTT assay was used to assay cell viability, the DCF-DA fluorescent probe to evaluate ROS induction, and cell-cycle analysis to measure the antiproliferative effect. Some of the compounds showed a certain degree of cytotoxicity towards all the malignant cell lines tested. In some cases, an induction of increased generation of ROS was found in HeLa cells. Therefore, these novel 1,4-naphthoquinone derivatives may be useful as antitumoral agents in the treatment of different cancers.

Biography

Gabriele Micheletti is currently assistant in the Department of Industrial Chemistry at the University of Bologna. His field of specialization is organic chemistry and he has completed his studies in Industrial Chemistry in 2006, at the Faculty of Industrial Chemistry University of Bologna, Italy. In the 2011 he has pursued his PhD in Chemical Sciences at the same University. His fields of expertise are synthesis of novel organic compounds, organophosphorus chemistry, studies on mechanisms of organic chemistry reactions especially through detection of labile reaction intermediates by NMR spectroscopy (heteronuclear, dynamic variable temperature). Recent interest is in synthesis of new organic compounds of possible interest in biological field. He has more than 60 research publications in peer reviewed international journals.

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STUDY OF THE SYNERGY BETWEEN VGO AND HDPE PYROLYSIS WAXES IN THE HYDROCRACKING OVER NiW-Y ZEOLITES CATALYSTS

Suní Rodríguez, David Trueba, Francisco Javier Vela, Iratxe Crespo, Roberto Palos, Alazne Gutiérrez and José María Arandes

University of Basque Country (UPV/EHU), Spain

Abstract:

The rushed transition from fossil fuels to green energies, together with the increase in fuel quality requirements by environmental legislation, has led the refineries to the urgent necessity of renovating themselves. These changes have come at the same time of a high demand of fuel products such as combustibles and plastics. One way of renovation is using their infrastructure as a waste refinery, blending the usual refinery feeds with the by-products of the fast pyrolysis of plastics. The main advantage of this alternative is the possibility of including refineries in circular economy plans.

To carry out this renovation, we need to develop catalysts capable of maximizing the yield of high quality fuels from the blend of feedstocks first. In this line of research, we have developed two NiW catalysts supported on Y zeolites. The chosen Y zeolites were CBV 712 and CBV 780, and the metal content were 4.8 wt% NiO and 24.2 wt% WO₃, aprox. We have characterized these catalysts by acidity and textural properties means. We have also tested the catalysts in the hydrocracking reaction with vacuum gas oil (VGO) with a high S content and with high-density polyethylene (HDPE) fast pyrolysis waxes, showing a good performance in both cases. We carried out the hydrocracking reactions in a semi-batch reactor at 420°C, 80 bar, 1300 rpm, catalyst to oil mass ratio 0.1 gcat gcharge⁻¹, and 2 h of reaction time, in which hydrogen was continuously fed into the reactor. The next step in this research line is to test these catalysts with a blend of both feeds, looking for synergies between the feeds in the hydrocracking reaction.

Biography

Suní Rodríguez obtained the Degree in Chemical Engineering in 2016, and the Master's Degree in Environmental Engineering in 2017, both in the University of Valladolid (UVa), doing my Final Project and my Master's Thesis in the VOC & Odour Treatment investigation group, obtaining the end of master's degree award. The results obtained in my Degree Final Project and my Master's Thesis allowed me to appear as a contributor in the publication "Ectoine bio-milking in methanotrophs: A step further towards methane-based bio-refineries into high added-value products". I continued my professional career in the business world for a while, returning to the university as a researcher in the Process Control and Supervision group in the UVa. Since December 2020 I am a PhD student at the University of the Basque Country in the Catalytic Processes and Waste Valorization Research Group through a predoctoral FPI contract granted by the Ministry of Science and Innovation. My research focuses on the optimization of the yield obtained of gasoline and diesel fractions by catalytic hydrocracking of a mixture of VGO-HDPE pyrolysis waxes.

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March 20-21, 2023 | Rome, Italy



PEROVSKITE NANOCRYSTALS- NOVEL MATERIAL FOR REAL APPLICATIONS

Subhadip Ghosh

National Institute of Science Education and Research, India

Abstract:

Perovskite nanocrystals (NCs) are coveted materials, gradually evolving as potential contenders for building blocks in application fields such as the production of low threshold lasers, colour converting phosphors, light emitting diodes (LEDs), and many others. Facile synthesis, low exciton dissociation energy, rich optical properties and long carrier diffusion length are the fundamental properties leading to their successful utilization in device applications. Extraction of multi-excitons from NCs before Auger recombination is a challenging task due to the faster Auger recombination timescale. Wasting of excess energy through cooling and/or Auger recombination before extraction fundamentally limits the efficiency of a device. In a recent contribution, we have shown NC composition (complexed with the simple molecular system) enables fast carrier transfer, even before the Auger recombination. Blinking of NCs is another drawback, detrimental to their real applications. Using fluorescence lifetime correlation spectroscopy (FLCS) we revealed the origin of blinking lies to the trapping/de-trapping of carriers within the dispersive defect states. In my talk, I shall briefly discuss our findings on the above topics.

Biography

Subhadip Ghosh is an associate professor at the National Institute of Science Education and Research (NISER), India. He obtained his PhD in 2009 under the guidance of Prof. Kankan Bhattacharyya at the Indian Association for the Cultivation of Science, Kolkata, India. Before joining NISER in 2012, he worked as a postdoctoral fellow with Prof. Paul F. Barbara (2009–2011) at the University of Texas at Austin, United States, and subsequently with Prof. Tahei Tahara at Riken, Japan (2011–2012). His current research focuses on the photo-physical properties of carbonaceous and perovskite nanocrystals, employing various ultrafast and single-molecule spectroscopic techniques

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March 20-21, 2023 | Rome, Italy



CLASSIFICATION OF CATALYSTS WITH MIRA21 MODEL IN HETEROGENEOUS CATALYTIC HYDROGENATION OF AROMATIC NITRO COMPOUNDS

Alexandra Jakab-Nácsa, Viktória Hajdu, Emőke Sikora, Ádám Prekob, László Vanyorek, László Farkas and Béla Viskolcz

BorsodChem Ltd., Hungary

Abstract:

Industrial catalyst development requires complex R&D work, as many other factors must be considered in addition to the performance of the catalyst such as sustainability or economic considerations. Comparison of special catalysts in case of a given reaction could effectively support the design and development of catalysts, industrial application, promotes the monitoring of research and development trends and summarizes the latest results.

The aim of the work is to establish a functional and practical mathematical approach, called Miskolc Ranking 21 (MIRA21) model of catalyst characterization, classification and thus bias-free comparison of each other. Catalytic hydrogenation of aromatic nitro compounds is a key step in the industrial process of polyurethane production. This research summarizes the catalysts of dinitrotoluene hydrogenation to toluenediamine and nitrobenzene hydrogenation to aniline reactions by MIRA21 model. This systematic overview provides a comprehensive picture of previous and newest research results.

The model is also suitable for providing industrial companies the opportunity to select the technically and economically optimal catalyst supplemented with economic and purchasing data. The data analysis performed during the model creation determined the extremely important parameters, that measurement which assist to choose the right catalyst. Thus, the number of experiments and measurements can be significantly reduced, without the risk of data loss.

Special thanks goes to Ministry of Innovation and Technology financed project 2020-1.1.2-PIACI-KFI-2020-00121, for the professional support. Prepared with the Professional Support of the Doctoral Student Scholarship Program of the Co-operative Doctoral Program of the Ministry of Innovation and Technology and technology financed from the National Research, Development and Innovation Fund.

Biography

Alexandra Jakab-Nácsa simultaneously carries out the thorough research work required by the academic sphere, revealing deeper connections and the goal-oriented development work demanded by industry. Her chemical engineering activity focuses on optimizations. She achieved significant results with this activity in the chlor-alkali industry, where she also worked on the removal of pollutants from the salt solution and the extraction of materials that can be used as raw materials for other industries. Recently, her attention has been focused on catalytic processes. She studied catalytic hydrogenation processes in detail, especially on nitroaromatic systems. As a result of her research, she created the general model for heterogeneous catalysts known as the MIRA21 model. The developed model helps in finding the optimal type of catalyst by ranking, classification and comparison of them. During her research work, she pays special attention to sustainability aspects. As research and development coordinator she is an active member of many sustainability projects.

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Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



PIEZOELECTRIC PROPERTIES OF THE [001]-TEXTURED (NA, K) NbO₃-BASED LEAD-FREE PIEZOCERAMICS AND THEIR APPLICATION TO PIEZOELECTRIC ENERGY HARVESTERS

Su-Hwan Go and Sahn Nahm

Korea University, South Korea

Abstract:

0.96(Na_{0.5}K_{0.5})(Nb_{0.93}Sb_{0.07})O₃-(0.04-x)BaZrO₃-x(Bi_{0.5}Ag_{0.5})ZrO₃[NKNS-(0.04-x)BZ-xBAZ] ceramics are well textured along the [001] direction using 3.0 mol% NaNbO₃ seeds. The textured-NKNS-0.02BZ-0.02BAZ thick film has a rhombohedral-orthorhombic-tetragonal (R-O-T) structure with a large proportion of the R-O structure (> 80%). This specimen exhibits the largest values for d₃₃ (805 pC/N) and d₃₃×g₃₃ (29.5×10⁻¹² m²/N), which are the largest d₃₃ and d₃₃×g₃₃ values of NKN-based piezoceramics to date. Therefore, it is an outstanding piezoceramic material for piezoelectric energy harvesters (PEHs). A PEH are fabricated using this specimen. The PEH shows a large power density (4.3 mW/cm³), which is the largest value among the PEHs produced by lead-free piezoceramics. Therefore, texturing is an excellent technique for improving the piezoelectricity of NKN-based piezoceramics.

Biography

Su-Hwan Go received the B.S. & M.S degree from Hoseo University, Asan, Republic of Korea. He is currently in toward the Ph. D degree in the Korea University, Seoul, Republic of Korea. His current research interest includes lead-free piezoelectric ceramics and their application to piezoelectric actuator and energy harvesters

European Congress on

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Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



METAL NANOSTRUCTURES FOR ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE

Sudip Barman

National Institute of Science Education and Research (NISER) Bhubaneswar, India

Abstract:

The hydrogen evolution reaction (HER) and hydrogen oxidation reaction (HOR) in aqueous medium are two fundamental reactions for the development of non-fossil energy storage and conversion devices. In the polymer electrolyte membrane fuel cell (PEMFC) carbon supported platinum (Pt/C) based catalysts are universally used in cathodes and anodes; however, the poor durability of Pt/C due to degradation of the catalyst in the strongly oxidizing environment prevents its widespread applications. It remains a great challenge to develop new electrocatalysts with superior activity and very high durability for the HER/HOR. This study involves the synthesis of metal nanostructures on nitrogen doped carbon (MNSs-N@C; M=Pt, Pd etc.) composite for their superior activity and high durability toward the HER/HOR in acidic and alkaline media. These MNSs-N@C electrocatalysts exhibited 3–5-time higher HER/HOR activity than that of commercial Pt/C in alkaline media whereas MNSs-N@C and commercial Pt/C catalysts are of similar HER/HOR activity. The stability tests of these catalysts were done through a large number of repeated potential cycles and long-term electrolysis. These confirmed the exceptional durability of these catalysts, which is much better than that of commercial Pt/C catalysts. Furthermore, these catalysts have also displayed superior HOR activity, measured by a rotating-disk experiment with a broad range of pH (0–14) in different buffer solutions. The HER/HOR activities of MNSs-N@C composite in different buffer solutions were correlated with the hydrogen binding energy (HBE) of the catalyst surface. The HER/HOR activity gradually decreases with an increase in the HBE as the solution pH increases.

Biography

Sudip Barman is an Associate Professor in School of Chemical Sciences, National Institute of Science Education and Research (NISER) Bhubaneswar, Odisha, India. He received his PhD degree from Indian Institute of Science (IISc), Bangalore, Karnataka, India. He joined NISER Bhubaneswar as assistant professor in 2009. His research interest includes design and development of nanostructured materials for electrochemical energy storage and conversion such as electrochemical water splitting, Supercapacitors, Sodium ion batteries, electrochemical CO₂ reduction etc.

ENHANCEMENT OF ELECTROMECHANICAL COUPLING FACTOR OF THE $(\text{Na}, \text{K})(\text{Nb}_{1-x}\text{Sb}_x)\text{-SrZrO}_3\text{-(Bi,Ag)ZrO}_3$ PIEZOCERAMICS FOR PIEZO-ELECTRIC ENERGY HARVESTER

Seokjune Chae and Sahn Nahm

Korea University, South Korea

Abstract:

The 3.0 mol% NaNbO_3 templates were utilized to texture the $0.96(\text{Na}_{0.5}\text{K}_{0.5})(\text{Nb}_{1-x}\text{Sb}_x)\text{O}_3\text{-}0.01\text{SrZrO}_3\text{-}0.03(\text{Bi}_{0.5}\text{Ag}_{0.5})\text{ZrO}_3$ [$\text{NK}(\text{N}_{1-x}\text{S}_x)\text{-SZ-BAZ}$] piezoceramics ($0.0 \leq x \leq 0.08$) along the [001] orientation and they were well textured with the large Lotgering factor ($\geq 98\%$). The $\text{NK}(\text{N}_{1-x}\text{S}_x)\text{-SZ-BAZ}$ textured piezoceramics ($0.0 \leq x \leq 0.08$) have the rhombohedral-orthorhombic-tetragonal structure. The textured $\text{NK}(\text{N}_{1-x}\text{S}_x)\text{-SZ-BAZ}$ piezoceramics ($0.0 \leq x \leq 0.08$) show the good ferroelectric characteristics and the relaxor properties increased with the increase of x . The sample with $x = 0.01$ shows large k_p value of 0.77, which is the largest k_p value of the NKN-based piezoceramics reported in literatures. The large k_p value can be explained by the large phase angle of this sample. The piezoelectric energy harvesters (PEHs) were produced using the textured $\text{NK}(\text{N}_{1-x}\text{S}_x)\text{-SZ-BAZ}$ piezoceramics ($0.0 \leq x \leq 0.08$). The PEH produced using sample ($x = 0.01$) shows the large output power density of 6.07 mW/mm^3 at resonance frequency because of the large k_p value of the sample ($x = 0.01$). This is the largest power density observed for PEHs fabricated using lead-free piezoceramics to date, indicating that the textured $\text{NK}(\text{N}_{1-x}\text{S}_x)\text{-SZ-BAZ}$ piezoceramic ($x = 0.01$) is a good candidate for the PEH.

Biography

Seokjune Chae received the M.S degree from Korea University, Seoul, Republic of Korea. He is currently in toward the Ph. D degree in the Korea University, Seoul, Republic of Korea. His current research interest includes lead-free piezoelectric ceramics and their application to piezoelectric actuator and energy harvesters

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March 20-21, 2023 | Rome, Italy



A CHARACTERIZATION OF Na_2MoO_4 , Na_2WO_4 AND THEIR SOLID SOLUTION

Alberto Ubaldini, Flavio Cicconi, Francesco Gennarini, Chiara Telloli, Fabio Borgognoni, and Antonietta Rizzo

ENEA, Italy

Abstract:

Sodium molybdate, (Na_2MoO_4), is a material of great importance for nuclear medicine, because ^{99}Tc is obtained from its solutions containing ^{99}Mo , which is probably the most important isotope for medical imaging. The principle is that the ^{99}Mo radioisotope decays into ^{99}Tc and by feeding specific generators ($^{99}\text{Tc}/^{99}\text{Mo}$) with mother solutions containing the first, solutions of the second can be obtained. The generators are columns normally containing alumina, (Al_2O_3), which fix the molybdate ion, (MoO_4^{2-}) but do not retain the pertechnetate ion (TcO_4^-). Then this is formed inside the generator by the decay process and can be eluted with ease. The synthesis and production, together with the characterization of sodium molybdate are evidently very important. Chemically, sodium molybdate belongs to the spinel class and is a rare example of a compound I-VI in this group. Sodium tungstenate is isostructural and also contains a hexavalent cation.

In this work we present an easy method for the synthesis of both, starting from metals, by the use of concentrated hydrogen peroxide, discussing the kinetic and thermodynamic aspects. In this way very pure final compounds can be obtained, as it has been proved by ICP-MS. Also, since they are isostructural, some solid solutions have been prepared.

The samples were characterized by Raman spectroscopy, IR, Electron Scanning microscopy (SEM) and X-Ray Diffraction (XRD).

Biography

Alberto Ubaldini is graduated in Chemistry with honors at the Genoa University and later he received his PhD in Chemical Sciences, with a special focus in materials science from the University of Genoa in 2001. He carried out scientific research in several Italian and international institutes and advanced laboratories in Italy, France, Japan and Switzerland. He has expertise in many different preparative and analytical techniques and he has experience in the chemistry and physics of solid state, In particular he knows the methods of solid-state synthesis and the processes necessary to obtain high-quality compounds, but at the same time I know less traditional synthesis methods such as high-temperature high-pressure (HTHP) synthesis. This led to the publication of numerous original articles in many excellent international scientific journals. Recently, he has recently become researcher at ENEA in the Division for Nuclear Safety, Security and Sustainability. He carries out study, analysis, research, development and qualification of technologies, methodologies, materials, processes and products, advanced design, supply of advanced technical services, transfer and diffusion of technologies and knowledge to the production system, to Institutions and citizens.

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



INTEGRATED VALORISATION OF PHOSPHOGYPSUM USING pH DEPENDENT PURIFICATION PROCESS

Hamza Chanouri, Khalid Agayr, El Mahdi Mounir , Rachid Benhida and Khaoula Khaless

Mohammed VI Polytechnic University (UM6P), Morocco

Abstract:

Gypsum is one of the biggest sectorial employers in the European Union (EU), within an estimated turnover of 7.7 billion EUR. However, the high demand on this resource increased the supply risk. Studies forecasted a severe gap between the demand and supply, up to 30 million ton per year in 2030. This enthused researchers to direct their work toward new alternatives in order to compensate the difference and ensure a steady flow of gypsum. One of the most promising alternatives is the phosphate-based products i.e., phosphogypsum (PG).

PG is a by-product obtained from phosphate rock processing by sulfuric acid. For decades, PG has been a source of environmental concern due to the massive amount produced thus far, i.e., 7 billion tons, with a current production rate of 200-280 million tons per year. Owing to the presence of impurities in PG their direct application as a substitute of natural gypsum was prohibited, which implies the necessity of a purification step before any attempt of utilization.

To address this challenging question regarding the purification of PG this research study focused on the development of an innovative technic based on staged valorization of PG using pH dependent purification process. After screening different parameters and monitoring the ionic conductivity of solutions, it was disclosed that a pH-dependent solubilization process, under alkaline conditions, in the presence of specified green chemical solvents allowed a high solubility of PG, up to 11.82 g/100 mL, reported as the highest in literature. Subsequently, a recovery of the purified PG by selective precipitation of calcium sulfate dihydrate (CSD) from obtained filtrates through pH adjustment was investigated. An abatement of 99.34% Cr, 97.15% Cd, 95.73% P_2O_5 , 92.75% Cu, 92.38% Al_2O_3 , 91.16% Ni, 74.58% Zn, 72.75% F, 61.43% MgO, 58.8% Fe_2O_3 , 56.97% K_2O , and 55.41% Ba was achieved. In comparison to other measures, this work provides a new idea of integrated processing of PG for sustainable PG and gypsum management.

Biography

Hamza Chanouri is a PhD student at Chemical and Biochemical Sciences, Green Process Engineering department at Mohammed VI Polytechnic University. His research studies concern the valorization and purification of industrial by-products e.g., phosphogypsum and phosphoric acid sludge.

European Congress on

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



EXTENDED STUDY ON DATA ANALYSIS FOR INVESTIGATING CHEMICAL PROFILES FROM MeOH CRUDE OF *Euphorbia milii* FLOWERS APPLYING GC-MS

Nurul Huda Abdul Wahab, Vannisree R. Arunachalam, Asnuzilawati Asari and Ahmad Nazif Aziz

Universiti Malaysia Terengganu, Malaysia

Abstract:

Euphorbia genus has been widely applied in mainly treatment of constipation, inflammation and diarrhoea. This is because they are reported to exhibit certain pharmacological activities such as anti-inflammatory, antimicrobial, antifungal, antidiabetic, and antitumor. The purpose of this research is identifying the chemical profiles and investigate the biological activities of detected compounds in *Euphorbia milii* MeOH crude (flowers) using GC-MS. In this study, methanolic *Euphorbia milii* (flower) extract was analyzed under GC-MS method to detect the presence of the secondary metabolites. A gas chromatograph (GC) directly coupled to the mass spectrometer system (MS) of an Agilent 5975C inert MSD with triple-axis detector was used to run GC-MS analysis. Through the analysis, 56 chemical compounds were identified from methanol extract of *Euphorbia milii*. Among the identified chemicals compounds, only 16 significant chemical compounds are being studied in this research. Three saturated fatty acid ester, four saturated fatty acid, one unsaturated fatty acid, one flavonoid, one phthalate ester, four terpenoids, one carboxylic acid anhydride and one carboxylic ester was further studied to identify their biological properties. The most notable biological activities exhibit by the detected chemical compounds are antimicrobial, antioxidant, anti-inflammatory, antifungal and antibacterial. *Euphorbia milii* flower do have the presence of bioactive that exhibit several pharmacological activities which contributes to medicinal field.

Biography

Nhuda has her expertise on the isolation and structure elucidation of bioactive compounds from plants and marines' sources that could potentially become new lead metabolites or active drugs. She been exposed to the tools such bioassay, LCMS, GCMS or NMR-guided fractionations for the purifying works on the bioactive constituents. Her basic idea is to start really small scale of plants and marines' sources, screening process, that will then be used to further direct to isolate natural products and continue with synthesis work if possible.

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



COMBINED APPLICATION OF RESPONSE SURFACE METHODOLOGY (RSM) AND ARTIFICIAL NEURAL NETWORK (ANN) BASED ON EXPERIMENTAL DESIGN (DOE) IN MODELING AND OPTIMIZATION HDS ACTIVITY

Fawzi. M. Elfghi

Libyan Petroleum Institute, Libya

Abstract:

The main purpose of hydrodesulfurization unit is to remove sulfur from gasoil/diesel fuel. In this work, the estimation capacities of the Response Surface Methodology (RSM) and Artificial Neural Network (ANN), to determine the catalytic hydrodesulfurization activity were investigated. The article presents a combined application between response surface methodology (RSM) and artificial neural networks (ANN) in the modeling and prediction of the HDS activity. In this study, ANN methodology showed a very obvious advantage over RSM for both data fitting and estimation capabilities. Based on the results of analysis of variance (ANOVA), a multiple determination coefficient of 0.8 and 0.98 were obtained for both RSM and ANN respectively. It has been found that by employing RSM approach coupled with ANN model based on DOE strategy, the visualization of the experimental points in three dimensional spaces can disclose qualitatively and quantitatively the activity relationship.

Biography

Fawzi M. Elfghi is an Assistant Professor specialized in smart and advanced materials for Energy and Environmental applications. His main field in undergraduate and graduate studies was in Chemical Engineering. Process simulation, modeling and optimization of industrial processes of their variables and material structure using DOE, ANN and RSM strategy is one of his major contributions among his research record. Dr Fawzi published more than 25 technical papers and two books related to his research field in reputable publisher houses of ISI and Scopus indexed journals with impact factors. Dr Fawzi participated and contributed in more than 30 local and international conferences, symposiums, seminars and workshops. His H-Index is 9 with more than 400 citations since 2014.

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



RECOVERY OF RARE EARTH ELEMENTS FROM PHOSPHORIC ACID USING ION EXCHANGE RESIN

Anasse Sraidi , Sara Ait Hak, Khaoula Khaless and Rachid Benhida

Mohammed VI Polytechnic University (UM6P), Morocco

Abstract:

Rare earth elements (REEs) are a group of 17 elements, i.e., the group of lanthanides plus scandium and yttrium. Nowadays, REEs emerged as critical materials in the development and maintenance of industrialized economies. They are used in a range of high-tech applications, including super-magnets, smart phones, reactor components, smart batteries, hybrid cars, etc. During the two last decades, the market of REE is dominated by China as the first worldwide provider, with more than 90% of the world supply. The largest ores of REEs are estimated to occur in China with around 36%, followed by the Commonwealth countries (19%) and United States (13%). However, the limitation of recovery of REEs from primary resources makes their access from other secondary sources a real challenge to balance the supply crisis and to address the increasing market demand. Therefore, very recently, several countries are investigating the extraction of REEs from industrial side products and waste coming from high-tech material industry. Furthermore, phosphate rock as well as its transformed products and byproducts are known sources of REEs. Indeed, leaching of phosphate ore using wet process produced phosphoric acid and gypsum, both contain REEs at different concentrations. In this work, we investigate the recovery of REEs from phosphoric acid using macroporous exchange resin. Several parameters were studied to optimize the extraction efficiency such as the contact time, resin selectivity, acid concentration, temperature, as well as the kinetic and the thermodynamic of the process. The resin thermal stability and resin regeneration conditions for further cycles were also investigated. Other resin properties were also studied using FT-IR, SEM and TGA.

Biography

Anasse Sraidi is a PhD student at Chemical and Biochemical Sciences, Green Process Engineering department at Mohammed VI Polytechnic University. His research studies concern Phosphoric acid, Phosphogypsum, Extraction and separation process, Purification technologies , trace elements, rare earths and waste management.

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



ECOFRIENDLY SYNTHETIC PATHWAY FOR BIOINSPIRED METALLO MACROCYCLES: A NEW PARADIGM IN APPLIED CHEMISTRY

Ashu Chaudhary

Kurukshetra University, India

Abstract:

The varied nature of the chemical world requires various greener pathways in our quest towards attaining sustainability. Green chemistry has come a long way since its birth in 1991, growing from a small grassroots idea into a new approach to scientifically-based environmental protection. The emerging area of green chemistry envisages minimum hazard as the performance criteria while designing new chemical processes. Rather than end-of-the-pipe remediation approach, which involves cleaning up of waste after it has been produced, the main objective is to avoid waste generation in the first place. There are different shades of greener processes being developed as we continue exploring alternatives to conventional chemical synthesis and transformations. The desired approach will require new environmentally benign syntheses. The chemistry of macrocyclic complexes has witnessed an outline by individual scientific backgrounds and individual interest due to their analytical, industrial, agricultural and medicinal. The anticancer properties of square-planer platinum compounds have fueled an interest in the chemistry of all the metal complexes. Keeping all these factors in mind we aimed to synthesize and characterize macrocyclic compounds with N_4 -tetraamide ligands. The main emphasis has been given on in vivo studies on male rats by performing biochemistry and fertility test. The aim is also to prevent the toxic effect or abnormal observations of the pesticides and antifertility agents. Good antimicrobial complexes have been selected for antitumour activity. The positive findings will be discussed in detail.

Biography

Ashu Chaudhary is Assistant Professor of Chemistry, Kurukshetra University, Kurukshetra. She has research/teaching experience 17 years with specialization in Green Chemistry and Bioinorganic Chemistry. Dr. Chaudhary's pioneering contributions have strongly influenced on Metal Based Drug designing and Nano particles in Cancer Therapy. She proposed that solvent reorganization in metal ligand interactions in general underlie their specificity. Her original strategies for drugs design are widely acclaimed.

In her research functional materials have been wisely constructed via bottom up approaches as seen in synthesis of molecular patterns and complexes, organized nanostructures and function bulk materials. In addition, novel concepts "hand-operating nanotechnology" to bridge nano (molecular) structures and bulk systems is also initiated. These strategies enable to construct supramolecular structures, some of which are highly useful for bio related applications such as drug delivery and sensing. Dr. Chaudhary has reported ecofriendly synthetic route of novel bio-organometallic complexes possessing pesticidal properties. Moreover, Dr. Chaudhary has synthesized the substitute of widely used pesticide D.D.T. (well-known for controversial history and banned due to high toxicity in 1972 for agricultural use).

She has authored more than hundred seventy publications in National and International journals of high impact factor including review articles and book chapters. Her contribution to Bioinorganic chemistry have been recognized widely. Dr. Chaudhary is a recipient of Glory of India Gold Medal-2016, Bharat Gaurav Award-2016, Research Excellence Award-2016, Outstanding Faculty Award-2016, Bharat Gaurav Award-2015, Eminent Young Scientist of the Year Award 2015, Rajasthan Gaurav-2015, Rajiv Gandhi Excellence Award-2015, Outstanding Scientist Award-2015, Best Researcher Award-2015, Swashakti Samman-2015, 6th Rajiv Gandhi Excellence Award-2015, Young Scientist of The Year Award-2014, Environmentalist Of The Year Award-2014 and Eminent Scientists of the Year Award 2010 by National Environmental Science Academy, New Delhi. Her research work were recognized through several awards that include Young Scientist Award-2009 by Indian Council of Chemists at Patan, Gujrat, Scientist of the Year Award-2009 by National Environmental Science Academy, New Delhi, and Sudesh Bhasin Memorial Award-2008 by Indian Council of Chemists at Haridwar, Young Scientist Award-2008 of International Conference on Green Chemistry, S.G.B. Amaravati University, Amravati, Young Scientist Award-2005 of International Conference on Sustainable Development and Resource Utilization: Current Trends and Perspectives in Jaipur.



Day 2

**Chemistry Congress
&
Catalysis
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Keynote Presentations

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



HYDROGEN, AMMONIA, CCU AND BEYOND – ELECTRIFICATION OF INDUSTRIAL UNIT OPERATIONS



Blaž Likozar

Kemijski inštitut, Slovenia

Abstract:

The current climate, health and economic condition of our globe boundaries demands the use of renewable energy sources, harvesting, and the development of the abundant novel materials for an efficient generation, storage and transportation processes of this sustainable energy. Hydrogen has been recognised as one of the most prominent chemicals, carriers and a green energy source with a challenging pressurised storage, enabling de-carbonization. Electro- or photocatalytic H₂ (renewable green hydrogen) production processes are targeting the intensification of separated solar energy harvesting, storage and electrolysis stages, conventionally yielding O₂/H₂.

To address storage, the conventional large-scaled method for synthesizing ammonia is a power-hungry process that requires a high operating temperature (400-500°C) in addition to extremely elevated pressures (150-300 bar). Reaction is normally catalysed by magnetite-based material particles, is known for quite some time, and occurs between a single stoichiometric mole of nitrogen, three mole of hydrogen and energy to form two mole of ammonia. The original Haber–Bosch production process was discovered, developed and patented in 1916 by Fritz Haber and Carl Bosch, but is bound to be subjected to reengineering.

Analogously apply with the power to gas or liquid, where high performance computing enables optimisation. There has been a growing persistent trend to couple the different temporal/spatial levels of modelling, such as going from the first principle calculations to meso- (e.g. kinetic Monte Carlo, KMC), and macro- (e.g. computational fluid dynamics, CFD) and planetary boundary scale. In current multi-scalar investigation, a CFD study of the CO₂ hydrogenation to methanol for the heterogeneous reacting flows in the reactors with complex shape geometries is put forward, coupled with first principle calculations (density functional theory, DFT).

Biography

Blaž Likozar is a Head of the Department of Catalysis and Chemical Reaction Engineering at the National Institute of Chemistry (NIC), leading the programme “Chemical Reaction Engineering”, as well as numerous research projects (15 H2020 / 23 in Horizon Europe alone). His expertise lies (among others) in heterogeneous catalysis materials, modelling, simulation and optimization of process fluid mechanics, transport phenomena and chemical kinetics. He worked at the University of Delaware in 2014–2015 as a Fulbright Program researcher. He has authored >290 articles, was cited >5000 times, having a h-index of 38.



Day 2

**Chemistry Congress
&
Catalysis
2023**

Oral Presentations

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



EVALUATION OF THE EFFICIENCY OF COAGULATION- FLOCCULATION PROCESS FOR TREATMENT OF TEXTILE WASTEWATER USING A NATURAL FLOCCULANT - CACTUS *Opuntia Ficus Indica*

Belkacem Merzouk, Billal Khemila, and François Lopicque

University of M'sila, Algeria

Abstract:

The use of natural flocculant in coagulation-flocculation (CF) treatment of wastewater shows many advantages over chemical agents, particularly biodegradability, low toxicity, low residual sludge production and low-cost. In this work, the ability to remove a synthetic and a real textile wastewater using CF process with aluminum sulfate $Al_2(SO_4)_3$, ferric chloride ($FeCl_3$), industrial (anion) flocculant and a mucilage of *Opuntia ficus indica* as a natural flocculant aid has been investigated. Results showed that:- The stirring velocity for coagulation must be fast in a time of very short mixture (150 rpm - 3 min). - The stirring velocity of flocculation must be slow in a time of average mixture (30 rpm - 20 min). - CF functions well, even with the highest dyestuff concentrations, going up to 600 mg/L (1959 NTU) for aluminum sulfate ($\gamma_{Turb} = 99\%$) and 800 mg/L (2717 NTU) for ferric chloride ($\gamma_{Turb} = 96.83\%$) under initial pH ranging from 8.5 to 10.5. - The optimal amount of ferric chloride and aluminum sulfate is of 250 mg/L. - The optimal amount of the anion flocculant for the elimination of turbidity with aluminum sulfate is 50 mg/L, and that of ferric chloride is 5 mg/L. - The optimal amount of the natural flocculant agent is 12 to 15 mL/L. - By adding 3 ml/L of *Opuntia ficus indica* as a natural flocculant aid, the efficiency increased by 10 %. - The application of the optimized parameters to a real textile wastewater showed an acceptable reduction of the turbidity (67 %), SS (57.33 %) and COD (94.81 %).

For all these reasons, it can be concluded that the use of cactus *Opuntia ficus indica* as an aid flocculant can be recommended to improve the efficiency of the CF process for the treatment of textile wastewater.

Biography

Belkacem Merzouk (49 years) has completed his PhD since 2009 from Bejaia University (Algeria). He obtained his HDR in 2011 at Bejaia University. He is a professor since 2016. He is a teacher-researcher at M'sila University since 2004 (Magister). Since February 16, 2016 to June 14, 2022, he was the president of the scientific committee of the hydraulics department. He has supervised more than 14 engineers, 21 Masters and 7 PhD theses. He took part as member of examination committee in 9 Thesis and 5 HDR. He has published 21 papers in reputed journals. He has an h-index of 15 and 1888 citations (September 8, 2022). He is a reviewer for more than 15 highly ranked journals, and he is member or head in national and international research projects. He has been active in conferences as a member of organizing committees, scientific committees and invited speaker. His research interests lie broadly in the identification of innovative and cost-effective solutions within the fields of water resources and wastewater treatment including coagulation-flocculation, electrocoagulation.

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NEW APPROACHES TO SIMULATION OF ENZYMATIC REACTIONS: MIMETIC CATALYSIS

Tofik Nagiev

Nagiev Institute of Catalysis and Inorganic Chemistry, Azerbaijan

Abstract:

The area between enzymatic and chemical catalysis, associated with simulation of biochemical processes by their basic parameters, is accepted as mimetic catalysis. The key aspect of the mimetic catalyst is diversity of enzyme and biomimetic function processes, which principally distinguishes the mimetic model from traditional full simulation. Based on the analysis of conformities and diversities of enzymatic and chemical catalysis, the general aspects of mimetic catalysis are discussed. An idealized model of the biomimetic catalyst and the exclusive role of the membrane in its structural organization are considered. The most important achievements in the branch of catalysis are shown, in particular, new approaches to synthesis and study of biomimetic catalase, peroxidase and monooxidases reactions.

It is suggested that the catalysis approach, originating from the simulation of biochemical processes, is called 'mimetic catalysis'.

Mimetic catalysis designs a real model (a mimic) which simulates objects and processes of enzymatic catalysis by their basic (but deficient) characteristics (selectivity, mildness of condition, active site action mechanism, etc.). Since only definite properties of the enzyme are simulated, it does not profess to a complete enzyme description, though optimal parameters by some properties may be approached. The mimetic model of enzyme helps in synthesizing suitable catalysts using inaccurate and sometimes ambiguous information.

The overwhelming majority of biomimetics operate in liquid. Their activity depends on the origin of solvents, reaction mixture and cell effects. Gas-phase oxidation processes are less dependent on these effects and in the first approximation can be considered as oxidation under quasi-ideal conditions. It goes without saying that enzymatic reactions do not proceed in gases. However, it is possible to simulate catalytic functions in the gas phase. This simplifies the decoding of the reaction mechanism, not complicated by factors accompanying the liquid-phase oxidation.

Biography

Tofik Nagiev is a Vice-president of Azerbaijan National Academy of Sciences, Director of Research Center and Department chief of Nagiev Institute of Catalysis and Inorganic Chemistry of ANAS. The Professor of the department of the physical and colloid chemistry of Baku State University. He is author of the monographs "Coherent Synchronized Oxidation Reactions by Hydrogen Peroxide", Amsterdam: "Elsevier", p. 325, 2007; "Conjugated Reactions in Chemistry and Biology in the Context of Modern Ideas", "Generis Publishing", p.165, 2021.

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NEW SCHIFF BASE LIGANDS AND THEIR CORRESPONDING ZINC COMPLEXES. SYNTHESIS, CHARACTERIZATION AND COMPUTATIONAL STUDY

Taghreed MA Jazzazi

Yarmouk University, Jordan

Abstract:

Two new complexes (Zn1 and Zn2) were prepared by refluxing the new Schiff base ligands (L1 and L2) with Et_2Zn in THF solvent. The new ligands (L1 and L2) were prepared by reacting two equivalents of 3,5-dihydroxy-salicylaldehyde with two different amines which are 2,2'-diamino-4,4'-dimethyl-1,1'-biphenyl and 2,2'-diamino-6,6'-dibromo-4,4'-dimethyl-1,1'-biphenyl. The new Schiff base ligands and their zinc complexes were characterized by ^1H -, ^{13}C -NMR and IR spectroscopy as well as elemental analysis. The structures of all prepared ligands and their zinc complexes were resolved by X-ray structure determination. Additionally, their molecular geometries were fully optimized and examined using density functional theory (DFT) calculations at the B3LYP/6-31G(d) level of theory. Infrared vibrational analysis was conducted, and the results are in good agreement with the experimental data.

Biography

Taghreed Jazzazi is associate professor in chemistry department at Yarmouk University-Jordan. I have my expertise in synthesis and characterization of organometallic compounds. My research interest is metal organic chemistry, bioinorganic chemistry and CO-releasing molecules. I have built my experience after years of experience in research, and teaching both in my laboratory and the university.

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March 20-21, 2023 | Rome, Italy



UNDERSTANDING PROTEIN-SUGAR INTERACTIONS USING MOLECULAR MODELING TECHNIQUES

Madhumita Dandopath Patra

Acharya Prafulla Chandra College, India

Abstract:

Proteins form the very basis of life. They regulate a variety of activities in all known organisms, from transporting oxygen, to replication of the genetic code, and are generally responsible for regulating the cellular machinery and consequently, the phenotype of an organism. Functions of proteins are intimately connected to their three-dimensional (3-D) structures. In the post genomic era, the primary structures, i.e. the amino acid sequences, are available of a large number of proteins, in the sequence databases but the 3-D structures are known for a very small number of proteins. A major goal of structural biologists is to predict the 3-D structure from the amino acid sequence of a protein which would enhance the understanding of protein-ligand interactions. Carbohydrates are the most abundant of the four major classes of biomolecules, which also include proteins, lipids and nucleic acids. They have numerous roles in living things, such as the storage and transport of energy (glycogen, starch) and structural components (chitin in animals, cellulose in plants). Additionally, carbohydrates and their derivatives play major roles in the working process of the immune system, pathogenesis, fertilization, blood clotting, and development. Many carbohydrates reversibly bind to a wide variety of proteins with high specificity. These proteins may serve as drug targets because of their essential roles in the attachment of pathogenic organisms to the host cells. The specificity of binding to the terminal sugar moiety is determined by the chemical forces involved in the formation of complexes of these sugars with the amino acid residues of the binding site. The protein-carbohydrate interactions have been investigated in recent years through the analysis of the 3-D structures of a number of proteins and their complexes with carbohydrates, by NMR spectroscopic and X-ray crystallographic methods as well as by molecular modeling studies.

Biography

Madhumita Dandopath Patra have spent my initial years in Bankura, a district town in West Bengal, India. I graduated from Bankura Christian College in 2000 with Chemistry honours and secured first place amongst all streams of the College. My hard work and perseverance helped me win the Sachhidananda Gold Medal, 2000, P.C .Roy Memorial Scholarship, 2000 and the National Scholarship, 2000. After that I did my postgraduation in Chemistry with Organic chemistry as a special paper, from University of Burdwan, 2002. Here I won the Bronze medal for achieving highest marks in Organic Chemistry, 2002.

After qualifying for UGC -CSIR NET, I completed my Ph.D. from Indian Institute of Chemical Biology (IICB), 2008, Kolkata. Herein my research was based on "Structural studies on Protein- Carbohydrate-interactions and inhibitor design using molecular modeling techniques ". I did my Post doctoral research in the field of "Protein Crystallography" from Saha Institute of Nuclear Physics, Kolkata in 2009. In 2010, I got an opportunity, to work as an Assistant Professor in the Department of Chemistry, Acharya Prafulla Chandra College, under West Bengal State University, India. My teaching involves both Post graduate and Under graduate students in the field of chemistry and I am also continuing with research work in the field of Structural Biology and Theoretical Chemistry.

My passion for research in science helped me to publish 11 research papers with 9 of them as lead author, in reputed International journals and I have also presented my work in several International and National seminars. I am also involved with lots of administrative work in my college. I have been appointed a member of board of Post graduate studies, convener of women's cell and member of examination committee etc.

To add further I am also acting as a reviewer of many international journals.

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



SYNTHESIS AND CHARACTERIZATION OF BORATE NANOPARTICLES

Alberto Ubaldini, Flavio Cicconi, Francesco Gennarini, Chiara Telloli, Fabio Borgognoni, and Antonietta Rizzo

ENEA, Italy

Abstract:

Alkaline earth metal borates are promising materials due to their many excellent properties which allow for applications in numerous fields. In fact, they have good thermal stability, excellent mechanical properties, excellent properties in the field of non-linear optics and in principle their nano particles can also be used as bacteriostatic and mycocides. Barium borate, BaB_2O_4 can find applications in the nuclear field, as it is a rare material which, containing both a light and a heavy element, can function both as a shield for thermal and high-energy neutrons and for X-ray.

However, these materials are difficult to produce in the form of micro and nano particles due to their chemical properties. Normally they are produced only by reactions in the solid state or by hydrothermal methods which lead to the formation of large particles.

This work proposes an alternative method, by controlled precipitation, for the formation of micro/nano particles of calcium, strontium, barium borates and their solid solutions, using borax as starting material.

The effects of experimental conditions, such as temperature, concentration, pH are discussed and a mechanism for the formation is proposed.

The particles were characterized by Raman spectroscopy, X-ray diffraction and electron microscopy. Furthermore, the synthesis of particles of other boron-containing systems is also presented, such as boric acid, which unlike the borates themselves is highly soluble in water. For these particles, innovative and alternative methods have been proposed. In particular, a sonochemical synthesis route supported by the presence of surfactants is presented, which could potentially be of general interest for many layered materials.

Biography

Alberto Ubaldini is graduated in Chemistry with honors at the Genoa University and later he received his PhD in Chemical Sciences, with a special focus in materials science from the University of Genoa in 2001. He carried out scientific research in several Italian and international institutes and advanced laboratories in Italy, France, Japan and Switzerland. He has expertise in many different preparative and analytical techniques and he has experience in the chemistry and physics of solid state, In particular he knows the methods of solid-state synthesis and the processes necessary to obtain high-quality compounds, but at the same time I know less traditional synthesis methods such as high-temperature high-pressure (HTHP) synthesis. This led to the publication of numerous original articles in many excellent international scientific journals. Recently, he has recently become researcher at ENEA in the Division for Nuclear Safety, Security and Sustainability. He carries out study, analysis, research, development and qualification of technologies, methodologies, materials, processes and products, advanced design, supply of advanced technical services, transfer and diffusion of technologies and knowledge to the production system, to Institutions and citizens.

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Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



SYNTHESIS AND ANTIBACTERIAL PHOTODYNAMIC ACTIVITY OF THE NEW PHOTOSENSITIZER 5,10,15,20-TETRAKIS(4-ETHYLPHENYL) PORPHYRIN

Fabián Espitia-Almeida, Roger Valle-Molinares , William Vallejo , Carlos Díaz-Uribe, Elkin Navarro-Quiroz, Leonardo Pacheco-Londoño and Nataly J Galan-Freyle

Universidad del Atlántico, Colombia, Universidad Simón Bolívar, Colombia

Abstract:

According to the WHO, resistance to antibiotics is currently the greatest global health threat, projecting to be the next pandemic, so the development and/or improvement of strategies to control the appearance of resistant microorganisms is a challenge and this must be approached from different points of view such as primary prevention and new antibiotics development. We evaluated the phototoxic potential of the photosensitizer 5,10,15,20-tetrakis(4-ethylphenyl)porphyrin (TEPP) against *Pseudomonas aeruginosa* (Pa), *Staphylococcus aureus* (Sa), and methicillin-resistant *Staphylococcus aureus* (MRSA). TEPP was synthesized following the Adler method, and characterized by UV-Vis, FT-IR, DRX, ^1H and ^{13}C NMR. We determined its quantum yield of fluorescence (ϕ_f) and singlet oxygen (ϕ_Δ). Through the microdilution technique, the phototoxic potential of five (5) concentrations of TEPP (5, 10, 20, 35, 50 $\mu\text{g/ml}$) was evaluated. Inhibition percentages and minimum inhibitory concentration (MIC) were calculated for each bacterium. An ANOVA and Tukey's post-hoc were applied to determine the differences between treatments ($p < 0.05$). The results suggest statistical differences between the irradiated and non-irradiated treatments with visible light, reaching the highest inhibition percentages at the concentration of 50 $\mu\text{g/mL}$ with 99.3, 93.4 and 81.7% for Pa, Sa and MRSA respectively; MIC values could not be calculated for non-irradiated treatments, suggesting that irradiation is necessary for to achieve effective inhibition. The MIC (R^2) values for the irradiated treatments were 35.9 (0.99), 22.8 (0.78) and 29.4 (0.97) $\mu\text{g/mL}$ for Pa, Sa and MRSA respectively. The TEPP photosensitizer was effective against the three bacteria evaluated in the study, presenting itself as a promising molecule that requires further studies in the future to understand its antibacterial behavior.

Biography

Fabian Espitia-Almeida is a chemist with a Master's degree in Biochemistry and PhD in Tropical Medicine. He currently works as a professor and researcher at the Simon Bolivar University located in Barranquilla, Colombia. He is part of the Center for Research in Life Sciences of the Simon Bolivar University and is attached to the Faculty of Basic and Biomedical Sciences of the same institution. His area of work includes chemical medicine, bio prospecting for medicinal purposes and biochemistry of disease (metabolic alterations related to obesity). Dr. Espitia-Almeida has nearly 7 years of research experience where he has published 14 original articles in national/international high impact journals and has participated in more than 10 national/international scientific events as a keynote speaker. She has extensive experience in the design of models for the evaluation of the biological potential of synthetic and plant extracted molecules (compounds) against various sensitive and resistant pathogens (bacteria, parasites, fungi and viruses). The model that we apply in this work is the effort of many years of dedication of our entire group.



Day 2

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&
Catalysis
2023**

Poster Presentations

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



SOLVENT-FREE IRIDIUM-CATALYZED SYNTHESIS OF SILYL CARBAMATES FROM THE REACTION OF AMINES WITH CARBON DIOXIDE AND HYDROSILANES

EA Jaseer, Francisco J Fernández-Alvarez and Luis A Oro

King Fahd University of Petroleum & Minerals, Saudi Arabia

Abstract:

Silyl carbamates were synthesized from amines, carbon dioxide and Hydrosilanes in the presence of catalytic amounts of the iridium (III)-NSiN complex, $[\text{Ir}(\text{H})(\text{CF}_3\text{SO}_3)(\text{NSiN})(\text{coe})]$ (NSiN=bis(pyridine-2-yloxy)methylsilyl). Iridium complex is proved to be effective catalyst precursor for the solvent-free synthesis of silyl carbamates and this work constitutes a first example using Iridium catalyst. The expected product from the reaction of amines, CO_2 and Hydrosilanes was formamide or methylamine. Interestingly, iridium-catalyzed dehydrogenative Si-N coupling between the silane and the amine was happened which afford the corresponding silyl amine. Then, silyl amine reacts with carbon dioxide under the reaction conditions to give the corresponding silyl carbamate. Theoretical and experimental calculations suggest that a competition between both hydrosilylation of CO_2 and dehydrogenative coupling reactions of amine-silane controls the selectivity of the process. Moreover, the size of the N-substituents on the amines plays a relevant role in the selectivity. Hence, for amines with bulky aliphatic substituents the dehydrogenative amine-silane coupling reaction is slightly hampered. In conclusion, we have found that in the presence of iridium complex, the dehydrogenative Si-N coupling pathway is preferred to the CO_2 -hydrosilylation pathway for mixtures of secondary aliphatic amines, carbon dioxide, and Hydrosilanes.

Biography

E A Jaseer, currently working as Associate Professor in the Center of Refining and Advanced Chemicals in the Research Institute at KFUPM, Saudi Arabia. I completed PhD at Indian Institute of Technology (IIT), Chennai, India in the area of homogeneous catalysis and asymmetric synthesis. I have joined King Fahd University of Petroleum & Minerals, Saudi Arabia as post-doctoral fellow, during which I have worked in the projects dealing with CO_2 utilization, polymer synthesis, synthesis of organometallic catalyst and its applications. After post-doc I was promoted to Research Scientist in the same university. My research work was focused on the utilization of the ligands like N-heterocyclic carbenes (NHCs), N-heterocyclic olefins (NHOs) to synthesize Iridium complex for several homogeneous catalysis like hydrogen transfer, hydrosilylation and hydroamination. Recently, I was focused in the area of oligomerization of ethylene using Cr/PNP complexes and polymerization of ethylene/alpha-olefin using metallocene and non-metallocene complexes. I have published more than 29 articles in peer-reviewed international journals and one US patent has been published. Moreover, I have presented many papers in national and international conferences and published one book chapter.

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



DESIGNING A LIGHT-UP PEPTIDE PROBE AS AN FID ASSAY INDICATOR FOR RNPs

Ujuagu Akunna Francesc, Lee En Ting Tabitha, Sato Yusuke and Nishizawa Seiichi

Tohoku University, Japan

Abstract:

The discovery of ribonucleoproteins (RNPs) and their role in viral replication and other cellular processes has sparked interest in the search for small molecule-based RNA binders as anti-viral agents. The fluorescent indicator displacement (FID) assay has been demonstrated to be a reliable tool for detecting new nucleic acid-binding ligands with a view toward the identification of RNP binders. While much effort has been put into developing FID indicators, it is still challenging to design the indicators with strong and selective binding affinity as well as large fluorescence signaling properties. Using the HIV-1 Tat protein-TAR RNA as a model, we designed a light-up peptide indicator (LUPI) containing the cyanine dye Thiazole Orange (TO). LUPI-TO gave a significant light-up response and a strong binding affinity of $K_d = 1 \pm 0.6$ nM upon binding with TAR RNA, demonstrating that it has promising potential as an FID indicator that can help screen for small molecules that bind to the TAR RNA.

To limit autofluorescence interference from the green spectral region of TO, we designed a fluorescent sensing probe with a deep red emission spectral range by incorporating benzo[c, d]indole quinoline (BIQ) into HIV-1 Tat protein-TAR RNA. BIQ-carrying LUPI has negligible emission in the absence of target RNA containing TAR RNA region, due to nonradiative energy loss because of free rotation of the benzo[c,d]indole and quinoline rings. The addition of target RNA caused a remarkable increase in the emission (> 1000 -fold) of the BIQ unit ($\lambda_{em} = 657$ nm), which indicates the intercalation of the BIQ unit upon binding of the peptide unit. In addition, we found that this probe had high selectivity for TAR RNA over noncognate RNAs such as bacterial A-site RNA and influenza A viral RNA. Considering that BIQ has a longer wavelength than TO, BIQ-carrying LUPI probe has promising potential as an FID indicator. We are hopeful that the LUPI concept will be applicable to other RNP complexes such as the N-protein/box B complex.

Biography

Ujuagu Akunna Francesc is a researcher with experience in experimental and analytical research on biological cells and tissues who is currently working on designing RNA-binding fluorescent indicators for high-throughput drug screening. She is currently a PhD student at the Department of Chemistry, Graduate School of Science, Tohoku University, Japan.

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



SILICA-SUPPORTED MONOALKYLATED TUNGSTEN DIOXO COMPLEX EXHIBITS CATALYTIC OLEFIN METATHESIS REACTION

Niladri Maity, Samir Barman and Jean-Marie Basset

King Fahd University of Petroleum & Minerals, Saudi Arabia

Abstract:

A well-defined silica-supported monoalkylated tungsten dioxo complex $[(\equiv\text{Si}-\text{O}-)\text{W}(=\text{O})_2(\text{CH}_2-\text{tBu})]$ was prepared by treatment of highly dehydroxylated silica ($\text{SiO}_2\text{-700}$: silica treated at 700 °C under high vacuum) with an ionic precursor complex $[\text{NEt}_4][\text{W}(=\text{O})_3(\text{CH}_2-\text{tBu})]$. The identity of the resulting neutral monoalkylated tungsten dioxo surface complex was established by means of elemental microanalysis and spectroscopic studies (IR, solid-state NMR, Raman, and X-ray absorption spectroscopies). The supported tungsten complex was found to act as a precatalyst for the self-metathesis of 1-octene in a batch reactor. The mechanistic implications of this reaction are discussed with the support of DFT calculations highlighting the potential occurrence of thus-far unexplored mechanistic pathways.

Biography

Niladri Maity, currently working as Research Scientist in the Center of Refining and Advanced Chemicals in the Research Institute at KFUPM, Saudi Arabia. I completed PhD from Indian Institute of Technology (IIT), Bombay, India in the area of Organometallic complex derived heterogeneous catalysis. I pursued my Postdoctoral Research from University of California Berkeley, USA (2008-2009); Institute for Molecular Science, Japan (2010-2013) and KAUST Catalysis Center, Saudi Arabia (2013-2017). I also served as Assistant Professor in Indira Gandhi Institute of Technology, Odisha, India (2018-2022). I have joined King Fahd University of Petroleum & Minerals, Saudi Arabia as a Research Scientist in 2022. My previous research experience was built on diverse expertise in design and development of homogeneous & heterogeneous catalysts focusing on surface organometallic chemistry, valorization of light alkanes (e.g., alkane metathesis, olefin metathesis, oxidative dehydrogenation of light alkanes, dehydrogenation of methane into aromatics and valuable chemicals), molecularly imprinted catalysts, homo- and hetero-bimetallic tandem catalysts, single-site catalyst, nanocatalysts. My current research work is focused on utilization of CO_2 into value added chemicals and synthesis of lubricant oil from alpha-olefin under homogeneous catalytic reactions. I have published 20 articles in peer-reviewed international journals including one book chapter.

DIAMONDOID HYDROCARBONS AS MATURITY INDICATORS FOR HIGH MATURITY CRUDE OILS AND CONDENSATES

Slavica Marinović and Mirna Biondić

INA – Industrija nafte Plc, Croatia

Abstract:

Thermal maturity is an important parameter in assessing petroleum evolution in sedimentary basins. The type of hydrocarbons generated (oil or gas) depends on the type of organic matter (type of kerogen) present in the rock, and to some extent, its maturation history. During sediment deposition, organic matter is exposed to elevated temperatures and pressures. The change of kerogen to petroleum under this condition over a long period is also known as maturation. These changes mainly include temperature reactions of cracking or pyrolysis (thermal cracking) of large molecules, and the formation of smaller molecules with lower energy content and increased stability. Determination of thermal maturity level of the organic matter source rocks and hydrocarbons in the reservoir is very important in source rock-oil correlation studies, and in solving the very complex problem of hydrocarbon migration from the source rocks to the reservoir rocks. Diamondoid hydrocarbons having the general molecular formula $C_{4n+6}H_{4n+12}$, are a class of saturated hydrocarbons that consist of three-dimensionally fused cyclohexane rings, which results in a diamond-like structure. Diamondoids show extreme thermal stability during exposure to high temperatures, therefore these compounds are used in the determination of thermal maturity of high maturity crude oils and condensates. These compounds are more stable than any other hydrocarbons, and once formed, are also resistant to biodegradation processes. Most “normal” oil samples have a high concentration of other biomarkers (hopanes and steranes), and a low concentration of diamondoids. Conversely, highly mature samples of crude oil and condensate generally contain a high concentration of diamondoids, and very low concentration of other biomarkers or in some cases are completely absent. During cracking to which hydrocarbons are exposed at high temperatures and pressures, diamondoids remain concentrated in condensate samples due to their extreme thermal stability compared to other groups of hydrocarbons. Diamondoid hydrocarbons were determined using gas chromatography-mass spectrometry in different concentrations and use of diamondoids as an indicator of the thermal maturity of hydrocarbons is based on different thermal stability of the methyl isomer of diamondoids.

Biography

Slavica Marinović completed her graduation in Chemistry in the University of Zagreb, Faculty of Chemical Engineering and Technology, 2001. She completed her Doctor of science, University of Zagreb, Faculty of Chemical Engineering and Technology, 2012.

Slavica Marinović is currently working as Senior Laboratory Expert in INA Oil industry,

Exploration and Production Laboratory, Zagreb (Croatia). She has over 20 years of experience working in an analytical laboratory dealing with oil and gas exploration and production. She is expert in Petroleum Geochemistry laboratory. Her research area includes source rocks evaluation and interpretation, chemical characterization of hydrocarbons (gas chromatography, gas chromatography-mass spectrometry, GC/MS, fossil fuel biomarkers, thin layer chromatography (TLC-FID), Rock-Eval pyrolysis, TOC, sulfur analysis etc.

Her research area also includes properties of petroleum products, biofuels, waste oil and sludge (UV/VIS spectroscopy, infrared and Raman spectroscopy, atomic absorption spectroscopy) etc. He has more than 20 professional and original scientific papers published in national/international journals.

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



ARYL-DI(PYRIDIL) PYRROLE GROUP IV COMPLEXES AS CATALYST IN ETHYLENE POLYMERIZATION

Nestor Garcia Villalta, Theodor Agapie, Muhammed Naseem Akhtar, E.A. Jaseer and Rajesh Theravalappil

King Fahd University of Petroleum & Minerals, Saudi Arabia

Abstract:

A variety of tris(dimethylamido) complexes $[(DPP^{Ar})M(NMe_2)_3]$ ($M = Ti, Zr, Hf$; $DPP^{Ar} =$ Aryl-substituted di(pyridyl) pyrrole, $Ar =$ mesitylene, anthracene), have been prepared by reaction of the pyrrole proligands with the corresponding $M(NMe_2)_4$ in Toluene at room temperature. X-ray quality crystals of $[(DPP^{mes})Ti(NMe_2)_3]$ were obtained by vapor diffusion of Pentane into a Toluene solution of the compound, Coordination of Ti to only two donors is observed pointing to the hemilabile character of the di(pyridyl) Pyrrolide ligands.

The catalytic activity in ethylene homopolymerization and ethylene-1-hexene copolymerization was Evaluated. Ti and Zr complexes were found to be competent when activated with $AlMe_3$ and $[CPh_3][B(C_6F_5)_4]$. The nature of the ligand system and metal centre affects the activities and PDI obtained.

Biography

Nestor Garcia is currently working as Research Scientist-III in the Centre for Refining and Advanced Chemicals (CRAC) in the Research Institute at KFUPM. He received his Ph.D. Degree in Chemistry, Master in Chemical Research and Bachelor of Science Degree in Chemistry from Zaragoza University, Zaragoza, Spain in 2013, 2010 and 2002, respectively. He is a member of American Chemical Society, Saudi Arabian International Chemical Sciences Chapter of the American Chemical Society and Royal Spanish Society of Chemistry

Dr. Nestor Garcia research contribution involves the synthesis and characterization by analytical and Spectroscopic means of non-commercial chiral ligands and optically active metal complexes, including the Molecular structure determination by X-ray diffractometric methods. Metal complexes containing have been tested as catalyst precursors in 1,3-Dipolar Cycloaddition, Hydrogen Transfer, Hydrosilylation as well as in the Diels-Alder reactions.

Dr. Nestor Garcia has published international refereed journal papers in reputed journals and has participated in national/international conference proceedings in the area of catalysis and polyolefin. His research work has been widely cited in scientific literature.

Dr. Nestor Garcia is actively involved in KFUPM in several projects related, ethylene oligomerization, ethylene and propylene polymerization and hydrogen transfer of aldehydes, ketones and imines catalysed bimetal complexes.

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



THE APPLICABILITY OF ROTATIONAL VISCOSITY IN SCOPE OF SAFETY ASSESSMENT OF AGROCHEMICALS

Kai Dollevoet

Charles River Laboratories, Netherlands

Abstract:

In safety assessment all types of chemicals ranging from industrial ones to pharmaceuticals can potentially be tested for various registrations. One example are agrochemicals, which are typically formulated mixtures, tested within the guidance of the Food and Agriculture Organization of the WHO (FAO).

Viscosity is a physico-chemical property that describes a substance's ability to absorb stress (translated shear stress), depending on the rate of deformation (shear rate). These parameters, show a viscosity relation that is linear for Newtonian liquids. When a substance consists of multiple constituents this can have an effect on the above relation, potentially causing a non-Newtonian behaviour, often not detected by various methods.. Therefore, the FAO recommends the rotational viscosity method, which has this applicability and can provide additional insight on the specific relation (e.g. dilatant, shear thinning, thixotropic, etc.).

In this method a sample is acclimatized at a set temperature, typically 20°C or 40°C, and retained in a container in which a concentric cylinder is immersed. At time of the measurement the cylinder will be rotating at a specified speed, representing the shear rate. During this period the shear stress of the sample on the cylinder is monitored as the torque of a coil spring. As described, the relation between these two parameters at different shear rates, provides information on the viscosity. The result can be used to assess the potential risks that the relation brings. For example, a dilatant solidifies under stress which could pose a danger when swallowed Or quicksand, which is a substance that allows shear thinning, which causes a reduction of viscosity under stress. Therefore, this method is the most suitable for the detailed safety assessment of this class of multicomponent agrochemicals.

Biography

Kai Dollevoet is Study Director at Charles River Laboratories in 's-Hertogenbosch, The Netherlands specialized in analytical and physical chemistry tests for safety assessment of products still in preparation of market sale. Within his expertise he and his colleagues look for better and safer methods for their assessments of materials in order to supply adequate results for sponsors and other stakeholders. Typical products for which examination is performed are: pharmaceuticals, agrochemicals, biocides and industrial chemicals. Apart from the viscosity testing presented, Kai and his team can provide testing over a wide range of guidance subjected to for example OECD, UN transport of Dangerous goods, EPA and analytical method development/validation following SANTE2020 or SANCO3030.

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SURFACE MODIFIED MESOPOROUS MATERIALS FOR PETROCHEMICAL REFINING PROCESSES

Sathiyamoorthy Murugesan

King Fahd University of Petroleum & Minerals, Saudi Arabia

Abstract:

The primary focus of surface organometallic chemistry (SOMC) has been on how organometallics react with surfaces comprising of highly divided and dehydroxylated oxides. Metal nanoparticle SOMC has been added to the field. Despite the fact that zeolitic materials are a specific class of oxides, SOMC has not, as far as we are aware, been applied to hierarchical fibrous zeolites. Hydrocarbon industrial chemistry benefits from zeolite catalysis. The sector still faces significant difficulties in finding the ideal balance between the activity and selectivity of zeolitic catalysts. The majority of the challenges stem from the abundance of surface sites, only some of which are catalytically active. Given that the petrochemical and refining industries are particularly dependent on the acido-basic characteristics and porosity of zeolites. Herein we present several surface modified materials [HZSM5-O-M(Np)₃, M = Ti, Zr, and Hf] that are supported on a hierarchical mesoporous H-ZSM-5 material. They are prepared utilizing SOMC concepts and resources. By carefully controlling the hydrogenolysis of [HZSM5-O-M(Np)₃], M = Ti, Zr, and Hf, materials, under H₂ (1 atm) at 150°C for 16 hours, they are further partially transformed into their corresponding metal hydride materials. Numerous spectroscopic methods, such as Fourier transform infrared spectroscopy, elemental analysis, solid-state NMR spectroscopy, powder X-ray diffraction, Brunauer-Emmett-Teller surface area measurements, scanning electron microscopy, and high-resolution transmission electron microscopy analyses, are used to characterize all of these surface catalysts. These clearly specified single-site materials will have their catalytic activity put to the test for petrochemical processes like hydrocracking distillates from crude oil or intermediate refinery process streams to useable petroleum products with added value for society.

Biography

Sathiyamoorthy Murugesan, currently working as Faculty in the Center of Refining and Advanced Chemicals in the Research Institute at KFUPM, Saudi Arabia. He completed PhD at Vienna University of Technology, Vienna, Austria in the area of Organometallics and Catalysis. He has done two-year postdoc with Rutgers University, NJ, the USA, followed by three-year postdoc with King Abdullah University of Science and Technology (KAUST), Saudi Arabia. His research interests include Novel material design for industrial applications, Hydrocarbon Conversion: hydro/cracking, and hydrodesulfurization, Sustainable Development: CO₂ utilization, Nitrogen fixation, Surface Organometallic Chemistry and its well-defined single/multiple-site Heterogeneous Catalysis, Zeolite Chemistry: well-defined Surface Functionalization / Modifications and its applications in Catalysis. He has published articles in peer-reviewed international journals and also filed many patents.

BIOLOGICAL EFFECTS OF HUMAN EXPOSURE TO ENVIRONMENTAL CADMIUM

Massimiliano Peana, Alessio Pelucelli, Christos T. Chasapis, Spyros P. Perlepes, Vlasoula Bekiari, Serenella Medici and Maria Antonietta Zoroddu

Università di Sassari, Italy

Abstract:

Cadmium (Cd) is a toxic metal for the human organism and for all ecosystems. Cd is naturally found at low levels; however, higher amounts of Cd in the environment result from human activities as it spreads into the air and water in the form of micropollutants as a result of industrial processes, pollution, waste incineration and electronic waste recycling. The human body has a limited ability to respond to Cd exposure, since the metal does not undergo metabolic degradation in less toxic species and is only poorly excreted. The extremely long biological half-life of Cd essentially makes it a cumulative toxin and chronic exposure causes harmful effects from the metal stored in the organs. The present paper considers exposure and potential health concerns on environmental cadmium with particular focus on its carcinogenic activity. Exposure to Cd compounds is primarily associated with an elevated risk of lung, kidney, prostate, and pancreatic cancer. Cd has also been linked with cancers of the breast and urinary bladder. The multiple mechanisms of Cd-induced carcinogenesis include oxidative stress with inhibition of antioxidant enzymes, promotion of lipid peroxidation and interference with DNA repair systems. Cd²⁺ can replace essential metal ions, including redox-active ones. A total of 12 cancer types associated with specific genes coding for the CD-metalloproteome were identified in this work. In addition, we summarize the proper treatments of Cd poisoning based on the use of selected Cd detoxifying agents and chelators, and the potential of preventive approaches to counteract its chronic exposure.

Biography

Alessio Pelucelli graduated at the University of Sassari in Pharmaceutical Chemistry and Technology in 2016, with distinction, presenting a thesis entitled 'Interaction of Ni(II) with peptide models of the TLR4 protein implicated in Nickel-induced allergic dermatitis'. The thesis was carried out under the supervision of Prof. Maria Antonietta Zoroddu and following an Erasmus experience at the University of Wroclaw (Poland), from which a collaboration with the research group of Prof. Elzbieta Gumienna-Kontecka was established. After graduation he spent a three-year period as a volunteer researcher in the field of NMR spectroscopy at the University of Sassari, where he then began his PhD in 2019 with a project entitled "Study and characterisation of peptide fragments involved in the formation of metal-protein complexes responsible in the pathophysiology of PCDD (Protein Conformational Disorders)".

His research work, carried out under the supervision of Prof. Serenella Medici, focused on the importance of metal ions (particularly transition metal ions) in the human body, and how these agents can positively or negatively influence the rearrangement of specific proteins involved in the development of pathologies. Through the NMR investigation of selected protein fragments, and by combining potentiometric studies, UV-Visible and EPR spectroscopies, and Circular Dichroism, it was possible to examine the coordination compounds that metal ions can potentially form under physiological conditions. The metal ions examined during this research work were predominantly Cu(II), Zn(II), Mn(II) and Cd(II), while peptide fragments were extracted from the hACE2 receptor and the FeoB operon. The latter was chosen and analysed in collaboration with the University of Wroclaw, where Alessio spent six months of his research period learning potentiometric techniques and applying them to his research work. The study of the FeoB operon has also allowed to expand the field of research to the interactions of metal ions (in particular Fe(II)) with bacterial proteins, laying the foundations for research aimed at a deeper understanding of these mechanisms with the purpose of paving new pathways in the interference with bacterial metabolism.

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CATALYTIC TRANSFORMATION OF RIBOSE TO FURFURAL IN PRESENCE OF HCL

Iwan Iwanov, Denitsa Yacheva and Nikolay Lumov

University of Chemical Technology and Metallurgy, Bulgaria

Abstract:

Ribose transformation to furfural is performed in water at heating in presence of conc HCl in portion to the water 7 : 18. To determine which hydroxyl group is protonated first in ribose molecule, we consider the structures of the four carbocations that form after protonation and dehydration of the four hydroxyl groups of ribose. Calculation of positive charge distribution and intramolecular binding energies were performed identifying carbocation 2 as the most stable followed by 1 and 3. Finally, with the lowest stability is carbocation 4, in which all four carbon atoms are on one side of the chain and the possibility of delocalization of the positive load is only in one direction. Explanation of full mechanism of open chain ribose to furfural. The reaction is going in 10 steps: Protonation of hydroxylic group, dehydration, deprotonation (giving back the catalyst) repeating three times (3 x 3) and cyclization to form a furfural ring; total 3 x 3+1=10 steps. Step 1. Protonation of HO-group corresponding to carbocation 2 which is the most stable and for that reason it appears first in reaction process. Step 2. Dehydration. The protonated HO-group forms a water molecule which leaves the ribose. Step 3. Deprotonation and restoration of the catalyst. Here stands the question: From which carbon atom deprotonation goes. We have two possibilities corresponding to two different reaction mechanisms. Step 4. Protonation of the next HO-group. Step 5. Dehydration. Step 6. Deprotonation and restoration of the catalyst. Step 7. Protonation of the final HO-group. Step 8. Dehydration. Step 9. Intramolecular nucleophilic attack and formation of furfural ring. Step 10. Deprotonation and restoration of the last catalyst. The same procedure was repeated in cyclic ribopyranose where only one possible mechanism was discovered.

Biography

Iwan Iwanov has experience in peptide synthesis (in solution and solid phase), drug design and discovery of new biological targets for cancer therapy; proposal writing including winning a funding of EUR 388 000 by the Bulgarian Ministry of Science. He has three peer-reviewed publications in three different journals on three different topics with three different research teams. During his teaching career in 2017-2019 Iwan Iwanov has discovered several unpublished and unreported on the net mechanisms one of them was ribose transformation to furfural. Iwan Iwanov has synthesized over 60 biologically active peptides published in Bulgarian Chemical Communications not referred by Scopus!

Funding: This research was funded by Ministry of Education and Science (Republic of Bulgaria), National Program "EUROPEAN SCIENTIFIC NETWORKS", project "Drug molecule", grant number D01-278/ 05.10.2020.

LTA PACKED BED MEMBRANE REACTORS FOR DME SYNTHESIS FROM CO₂ AND CO₂/CO_x MIXTURES: CRYSTALLIZATION OF THE MEMBRANE

Arancha Saiz Valderrama, Ainara Ateka, Onintze Parra, Ander Portillo; Javier Ereña and Andrés T. Aguayo

University of the Basque Country (UPV/EHU), Spain

Abstract:

The direct synthesis of dimethyl ether (DME) by the hydrogenation of CO₂ and CO₂/CO_x mixtures was studied in a packed bed membrane reactor. The role of the hydrophilic LTA zeolite membrane in this configuration is to remove H₂O from the reaction medium, reducing therefore the thermodynamic limitations of methanol synthesis and dehydration stages, as to promote DME production. The experimental work consisted of optimizing the crystallization of the LTA zeolite on the stainless-steel porous support of the reactor. The work was focused on selecting the most suitable materials for the synthesis of the membrane and the optimization of the crystallization method seeking for reproducibility. Two synthesis methods were studied with different reagents: (a) Preparation of the aluminate solution by adding 0.15 g pure aluminium beads (SigmaAldrich) to 25 mL deionized water containing 11.11 g sodium hydroxide (PanReac) at room temperature. The silicate solution was prepared by mixing 2.08 g LUDOX AS-40 colloidal silica (Sigma-Aldrich) and 23.75 g deionized water at 60°C under stirring. Afterwards, the silicate solution was added into the aluminate solution and stirred to produce a homogenous solution. (b) Preparation of the aluminate solution by adding 8.258 g sodium aluminate (Fisher-Chemical) to 40 mL deionized water containing 0.3615 g sodium hydroxide (PanReac). The silicate solution was prepared by mixing 15.48 g sodium metasilicate (Sigma-Aldrich) and 40 mL deionized water containing 0.3615 g sodium hydroxide. Afterwards, silicate solution was added into the aluminate solution to produce homogenous solution. Simultaneously, different crystallization times and temperatures were studied for both methods. The correct crystallization of the pursued zeolite was ascertained by SEM, XRD, NH₃-TPD and N₂ adsorption/desorption analyses. The experimentation determined that (a) synthesis method, performed at 70°C and 14.75h, is successful (99% purity) and reproducible for the synthesis of the LTA membrane on the porous support of the reactor.

Biography

Arancha Saiz Valderrama completed her graduate with a degree in Chemical Engineering (2019) by the Universidad Autónoma de Madrid and a Master's degree in Advanced Materials, Nanotechnology and Photonics (2020) by the same university. I did my Final Degree Project and Master Project at the Instituto de Cerámica y Vidrio (ICV, CSIC), where we did a research on the design of ceramics and composite materials for biomedical applications. In 2019 I participated at the VIII Conference of Young Researchers, organized by the Institute of Ceramics and Glass (ICV-CSIC), in the lecture: 'Hydrogel composites for use in bioinks for 3D-bioprinting of implants for bone tissue regeneration'. In January 2022 I joined the group Catalytic Processes and Waste Recovery (PROCAT-VARES) of the UPV/EHU with an FPI contract in order to study the selective production of olefins from CO₂, for the development of the doctoral thesis titled 'Application of the membrane reactor in the synthesis of hydrocarbons by CO₂ hydrogenation'.

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THE USE OF AFTER PRINTING PROCESS WASTE AS A FILLER FOR POLYMER MATERIALS

Krzysztof Moraczewski, Piotr Rytlewski, Magdalena Stepczyńska, Tomasz Karasiewicz, Magdalena Zaborowska, Bartosz Bolewski, and Alicja Suwała

Kazimierz Wielki University, Poland

Abstract:

The paper presents the results of the research on the possibility of using waste after the printing process as a filler for polymeric materials. Remains of the label backing were used, consisting mainly of cellulose with glue and polymer label residue. The properly prepared filler (washed, dried, pressed and cut) was added to the polypropylene in a volume ratio of 2: 1; 1: 1; 1: 2; and 1: 3 which corresponded to approximately 10; 5; 2.5 and 2 wt.% filler. Selected processing properties (mass flow rate), mechanical (tensile strength, impact strength, dynamic mechanical analysis) and thermal properties (thermogravimetric analysis, differential scanning calorimetry) were determined. Based on the research, it can be concluded that: the greatest decrease in polypropylene tensile strength after adding post-printing waste was 19% of the pure polymer value; the overall decrease in melt flow rate with the addition of most filler was 20% of the pure polypropylene value; the total decrease in unnotched toughness between the lowest and highest content of post-printing waste was 22%; the introduction of the post-printing waste into the polypropylene matrix did not change the thermomechanical characteristics of the polymer; the crystallinity melting of the tested materials decreased from 47.7% for pure polypropylene to 36.2% for the material containing a double excess of printing waste; The introduction of the post-printing waste into the matrix reduces the resistance by 17°C in relation to the value of pure polypropylene. The use of even the largest amount of filler did not cause disqualifying changes in the determined properties. The characteristics of the obtained materials allow them to be used in various applications, while reducing costs due to the high content of cheap filler.

Biography

Krzysztof Moraczewski is currently the Dean of the Faculty of Material Engineering at the Kazimierz Wielki University in Bydgoszcz. In his research work, he deals with issues of material engineering, in particular with regard to polymeric and composite materials. Currently, his research work is focused on the development of new and environmentally friendly polymer composites that will reduce the burden on the environment and fit in the framework of the circular economy. These activities are carried out in two ways. The first one involves the use of biodegradable polymers, which under special conditions of waste disposal quickly degrade, which significantly shortens the "life" time of pollutants. The second involves the use of post-production waste as fillers for polymeric materials, which can significantly reduce the amount of waste going to landfills. The remaining research areas concern the modification of the surface layer of polymeric materials, recycling of polymeric materials and electroless metallization of polymeric materials using classic electroless methods, as well as methods using biomimetic compounds.

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ENHANCED OIL REMOVAL AND REDUCTION OF ACTIVATED SLUDGE BY OZONATION EFFICIENCY OF A NEW MICROBUBBLE GENERATOR

Mory Traore, YaPing Ye, Aijun Gong, Yiwen Wang and Lina Qiu

University of Science and Technology Beijing, China

Abstract:

Sludge ozonation by microbubble generator technology, which promotes activated sludge reduction and oil removal, is promising for reducing waste sludge volume from petrochemical wastewater treatment. However, reducing the sludge with a small amount of ozone will be necessary if this technology is widely adopted. Therefore, we connected the microbubble generator to a gas-liquid mixer tube (linear mixer and Jet Pip mixer) to generate hundreds of nano ozone bubbles NOB and introduce them directly into the sludge suspension to enhance adhesion efficiency between oily flocs and nanobubbles and improve oil and sludge separation efficiency. As a result, within 120 minutes of ozonation for a dose of 0.3g O₃/g the mixed liquor suspended solids (MLSS) and the mixed liquor volatile suspended solids (MVSS) in sludge decreased by 55.8% and 24.02%, respectively. In addition, using a mixer coupled with H₂O₂ reduced the ozone amount and distinctly enhanced the oil removal; by 78.3% with NOB alone, 83.23% with NOB coupled with H₂O₂, and decreased the COD from 394.68 mg/L to 137.33 mg/l with NOB alone, and from 402.85 mg/L to 106.69 mg/l when coupled with H₂O₂. Combining a microbubble generator and a mixer produces ozone nanobubbles that persist in liquids for an extended time. Adding H₂O₂ to these fine ozone bubbles causes a highly effective reaction with target compounds in the activated sludge. The proposed method can cheaply perform activated sludge treatment while achieving environmental cleanliness and pollution reduction goals.

Biography

Mory Traore is working on synthesizing new rare earth nano-catalytic materials, studying the degradation behavior of polycyclic aromatic hydrocarbons (PAHs). In addition, he has expertise in waste treatment and improving global pollution issues.

PARAFFIN WAX IN PETROLEUM INDUSTRY: A REVIEW ON FORMATION, EXPERIMENTATION, PREVENTION, AND REMOVAL TECHNIQUES

Mirna Biondić and Slavica Marinović

INA – Industrija nafta PLC., Croatia

Abstract:

Crystallization of paraffin wax in crude oil, with subsequent deposition on the walls of pipelines and process equipment, is one of the main causes of many problems in the petroleum industry. Due to the paraffin wax deposition, there is a reduction in the actual diameter of the pipeline resulting in a higher pressure drops and the formation of gelled interlocking structures in the pipeline and process equipment, which leads to the interruption of crude oil production. There are two classes of petroleum waxes, paraffin wax and microcrystalline wax. Paraffin waxes consist of straight chain saturated hydrocarbons, with carbon atoms from C_{18} to C_{36} , crystallize in large flat plates, macrocrystalline structures. Waxes composed primarily of cycloalkanes and branched hydrocarbons, with carbon atoms from C_{30} to C_{60} , crystallize as small needle structures and are referred as microcrystalline waxes. There is two mechanisms of wax deposition, molecular diffusion, and shear dispersion. Molecular diffusion describes the process by which the radial temperature gradient in the line causes a concentration gradient of dissolved paraffin components in the liquid phase. Shear dispersion describes the relationship between deposition rate and shear rate.

Paraffin wax deposition can be prevented or removed by several different methods. These methods fall into three main categories: thermal, mechanical, and chemical. Laboratory analyses are carried out for the purpose of determining the tendency of paraffin wax deposition from crude oil. Paraffin wax analysis can include determination of paraffin wax content, molecular weight distribution, cloud point/pour point, wax appearance temperature, deposition test etc. Based on the composition of the crude oil, it is possible to predict the type of paraffin wax that will form and the best techniques for preventing and removing paraffin deposit from crude oil production system.

Biography

Mirna Biondić completed her graduation in Chemical Engineering in the University of Zagreb, Faculty of Chemical Engineering and Technology, 2010. Mirna Biondić is currently working as Laboratory Senior Expert in INA - Oil Industry, Exploration and Production Laboratory. The Exploration and Production Laboratory, based in Zagreb (Croatia), is dedicated to improve and support exploration, field development and oil and gas production. She has over 10 years of experience working in an analytical laboratory. She is expert in Fluid Characterization Laboratory. In the Fluid Characterization Laboratory, the physical and chemical properties of crude oil, gas condensate and petroleum products are determined (density, viscosity, pour point, flash point, water content, paraffin wax content, asphaltene content, acid number, FT-IR analysis, Cold Finger analysis). Her research area also includes determination of rheological properties of crude oil and testing flow assurance additives. The laboratory has a certificate according to the standard HRN EN ISO/IEC 17025:2017.

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LED-DRIVEN PHOTOCATALYTIC OXIDATION TECHNOLOGY FOR WATER PURIFICATION

Dan Gowland and Efthalia Chatzisyneon

University of Edinburgh, United Kingdom

Abstract:

Increased concentrations of natural organic matter (NOM), a complex mixture of organic substances found in most surface waters, have recently emerged as a substantial environmental issue. NOM has a significant variety of molecular and chemical properties, which in combination with its varying concentrations both geographically and seasonally, introduce the opportunity for an array of interactions with the environment. Due to an observable increase in amounts of NOM in water treatment supply sources, an improved effort to remove naturally occurring organics from drinking water supplies, as well as from municipal wastewater effluents, is required to continue the development of highly efficient and versatile water treatment technologies. Photocatalysis has received increasing interest from around the world, especially during the last decade, as several investigated processes have been regularly reported to be amongst the best performing water treatment technologies to remove NOM from drinking water supplies and mitigate the formation of disinfection by products. Consequently, this study investigates the optimised conditions for scaling up photocatalytic purification of drinking water using UV LED technology with TiO_2 based catalysts and compares the working conditions and limitations of possible photocatalytic drinking water systems.

The main objective of this study was to determine how affective photocatalytic treatment could be at treating NOM for drinking water purposes. Areas of focus in this study include testing various modified TiO_2 catalysts, organics concentrations & compositions as well as the possible applications of photocatalysis as a form of disinfection.

Biography

Dan's research career started out whilst completing his undergraduate course in Chemistry at Newcastle University during a year abroad at the University of Vermont. This research was based in organic synthesis and focussed on the creation of a novel synthetic pathway for a previously researched drug that would allow for easier testing of active site variants in 2 key areas. Dan's research career continued at Newcastle University when investigating a new technique for immobilising metallosurfactant dyes in mesoporous silica for various applications in photochemical and nanomaterial studies. This research project is what lead to Dan's interest in photochemistry and photocatalysis, eventually gaining a PhD research project sponsored by Scottish water at the University of Edinburgh under Dr Efthalia Chatzisyneon studying LED-driven photocatalytic oxidation technology for water purification. This project's day to day work includes testing of photocatalysts, photoreactor setup optimisation and the occasional E.coli disinfection investigation.

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RETENTION STUDY OF AN ORGANIC PERSISTENT MOLECULE BY SURFACTANT CLAY COMPOSITE (CLAY-C18TAB)

Abdelhak Mesbah, Imene Feddal, Safia Taleb and Monica Brienza

Djillali LIABES University (UDL) Algeria

Abstract:

Glyphosate an organic persistent pollutant, which widely used herbicide, is a significant environmental concern, the international agency for research on cancer IARC has classified glyphosate as a "probable carcinogen for humans". One approach to mitigating this contamination is through the use of clay materials for adsorption. Clay minerals, such as bentonite, have been found to effectively adsorb glyphosate from water due to their high surface area and ion exchange capabilities.

Studies have shown that the adsorption capacity of clay materials can be increased through various methods, such as modification with other adsorbents or through changes in pH. The purpose of this study is focused in the retention of glyphosate by adsorption on a surfactant clay composite (clay-C18TAB) and to study the influence of contact time, the mass of adsorbent and the pH of the solution on the removal efficiency.

The synthesized material was characterized by: PH_{PZC} , CEC (cation exchange capacity), FTIR (Fourier-transform infrared spectroscopy) and XRD, MEB-EDX.

The results showed that the material developed during this work has proven its effectiveness, it can be used in the elimination of glyphosate from water.

the use of clay materials for glyphosate adsorption is a cost-effective and eco-friendly solution compared to other methods, such as reverse osmosis or activated carbon filtration.

Biography

Abdelhak Mesbah a PhD student in analytical chemistry at university of Djillali Liabés Algeria on the subject of Experimental and analytical study of the retention process of organic pollutants by clay materials: case of herbicides : Diuron and Glyphosate, I am currently member of two research projects the first SAFE, PRIMA-2021 is focused in improving Safety in Agriculture, Food and the Environment, the second PRFU-2022 focused in the Experimental and theoretical study of the pollutant retention process by clay, I had some participation in doctoral day, national and international conference.

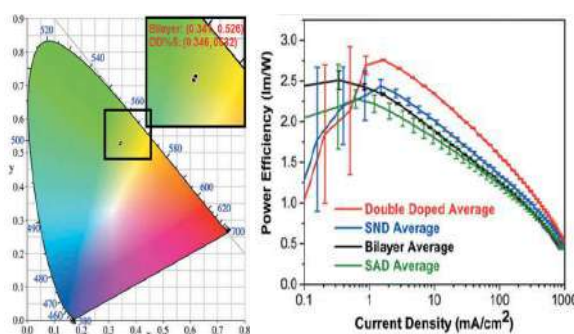
FABRICATION AND OPTIMIZATION OF A BILAYER ORGANIC LIGHT EMITTING DIODE DEVICE USING DOUBLE-DOPED LAYERS

Abdel-Monem M Rawashdeh, Mustafa Kharma, Dieaa Alhmoud, Aya AlHaj Issa, Ahmad Diabat, Aya Khatatbeh and Mohammad A Omary

Yarmouk University, Irbid, Jordan

Abstract:

A novel of structures OLED devices of the green-fluorescent main-group complex tris-(8- hydroxyquinoline) aluminum (Alq3). The standard bilayer devices was enhanced by including a double doped structure into the emissive region consisting of 20 nm *N,N'*-diphenyl-*N,N'*-bis(1,1'-biphenyl)-4,4'-diamine (NPB) and 10 nm Alq3 utilized as buffer layers for facilitating charge injection from the electrodes, and a broad emissive region stacked by two doped layers with a 5% Alq3 doped in a 50-nm thick NPB layer – as well as a 5% NPB doped in a 40-nm-thick Alq3 layer from the anode side to the cathode side. The double-doped device achieves a decreased turn-on voltage of 2.44 V and maximum brightness of 17,300 cd/m² as well as enhanced electroluminescence efficiency and moderately reduced efficiency roll-off over single-doped and standard





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APPLICATION OF ETHYLCELLULOSE-BASED SORBENT FOR SOLID-PHASE EXTRACTION FOR QUANTITATIVE DETERMINATION OF BENZOIC ACID IN MEDICINAL PRODUCTS

Tatyana Ryazanova, MN Kachalkin and AV Voronin

Samara State Medical University, Russia

Abstract:

An analytical procedure for the determination of benzoic acid in multicomponent medicines (Acerbine solution for external use, Caffeine and sodium benzoate tablets and solution for injections) using solid-phase extraction and UV-spectrophotometry has been developed. For solid-phase extraction, an ethylcellulose sorbent obtained according to the author's method (Kachalkin MN, Voronin AV. Preparation of sorbents for solid-phase extraction of salicylic acid from aqueous solutions. *Aspirantskiy Vestnik Povolzhiya*. 2021;(5-6):16–22. DOI: <https://doi.org/10.55531/2072-2354.2021.21.3.16-22>) was used. The selectivity (specificity) of the method with relation to other components of the studied medicines and certain aromatic organic acids (salicylic, 4-aminobenzoic, 4-nitrobenzoic, 2,4-dichlorbenzoic acids) in model mixtures was demonstrated. The specificity of the method was achieved due to selective binding of the analyte to active centers in the sorbent and step elution with purified water and 0.1 M sodium hydroxide solution in the course of solid phase extraction. Sorption capacity of the sorbent was 32.2 µg benzoic acid /g sorbent. The metrological characteristics of the developed technique for quantitative determination of benzoic acid were determined. The use of ethylcellulose-based sorbent makes it possible to improve metrological parameters and reduce the systematic error of the quantification procedure by an average of 40%.

Biography

Tatyana Ryazanova is currently working as an associate professor and a head of scientific and educational center "Pharmacy" in Samara State Medical University, Samara, the Russian Federation. Her field of specialization is Analytical Chemistry, Pharmacognosy and Economics in Pharmacy. She completed her specialist programme in Pharmaceutical sciences in 2011 with gold medalist / appreciation in Samara State Medical University and received a Ph.D. in Pharmaceutical Sciences (2015). Her field of expertise is standardization of medicines, including herbal plants/ herbal formulation. Her research area includes development of analytical procedures (UV-spectrophotometry, high-performance liquid chromatography), pharmacognostical & phytochemical investigation of Russian medicinal plants. She has 120 research/review publication in national/international journals, 15 patents and delegated more than 20 National/international conferences /workshops. She is honoured with young research scientist award by Samara oblast in the Russian Federation and she is awardee of a Scholarship of the President of the Russian Federation for young scientists and graduate students carrying out promising research and development in priority areas of modernization of the Russian economy".

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MAKING ETHYLENE-ALPHA OLEFIN ELASTOMER: INVESTIGATION OF LIQUID PHASE CATALYST ACTIVE CENTER RESIDENTIAL ENVIRONMENT AND NEW RESULTS

Muhammad Atiqullah

King Fahd University of Petroleum & Minerals, Saudi Arabia

Abstract:

Ethylene-alpha olefin elastomers are gaining versatile new applications and growing markets. Here, a solution copolymerization process makes elastomers using particularly alpha olefin-rich comonomer feeds, and metallocene and postmetallocene precatalysts. Copolymerization trials are conducted at laboratory to industrial temperatures and pressures, and they need the solubility of ethylene in the solvent-alpha olefin mixture. Therefore, this study models ethylene solubility in toluene-1-hexene and n-hexane-1-hexene mixtures under the above conditions. The model was developed using Peng-Robinson EoS and *vdW1f* mixing rule, Flory-Huggins interaction parameter, and Shulgin's activity coefficient-Henry's constant formalism. It, unlike those reported in the literature, eliminates cumbersome a priori assumptions and iterative calculation of vapor-liquid phase fraction, bubble point, and dew point, and calculation of liquid phase fugacity coefficient. Hence, it is more advantageous. The model-predicted ethylene solubilities in toluene, n-hexane, and 1-hexene well match the experimental values at laboratory to industrial temperatures and pressures (Part I). Part II uses Part I results, and well predicts ethylene solubility in solvent-alpha olefin mixture.

Modeling ethylene solubility also correlates the liquid phase mixture fluid compressibility to catalyst active center residential environment. This creates a new approach to investigate catalyst phenomena such as structural effect, activation, deactivation, and stability, as well as copolymerization phenomena, for example, monomer saturation and starvation, mechanism and kinetics, monomer reactivity ratios, micromixing effects, etc. Both phenomena can be now studied using a common footing. This is, therefore, a special contribution of this study to the literature.

This work addresses the above catalyst and copolymerization phenomena, as well as ethylene-1-hexene elastomer process development. The current practice of calculating kinetic model parameters, copolymerization reactivity ratios, and microstructural property such as sequence length distribution, using the solubility of ethylene only in the solvent such as toluene or n-hexane and ignoring that in 1-hexene, is significantly erroneous. The present work corrects it and solves a long-standing polymer reaction engineering problem.

Biography

Atiqullah is a Senior Research Engineer and Professor at the Interdisciplinary Research Center for Refining & Petrochemicals (IRCRAC), Research Institute, King Fahd University of Petroleum & Minerals, Saudi Arabia. He obtained his PhD in Chemical Engineering, studying at Columbia University and Rensselaer Polytechnic Institute (RPI), NY, USA. He is Editor-in-Chief at Research and Development in Materials Science Crimson USA. He is currently guest editing a special polyolefin issue in a Q1 polymer journal (IF = 4.967). He is a reviewer in 25 ISI journals. He is a recipient of several KFUPM awards. He is the lead inventor 6 US patents. He has 50 publications in Q1/Q2 journals. He is a regular keynote lecturer in his research area and a Japan Petroleum Institute (JPI) research fellow. He has successfully managed research projects for BASF The Chemical Company, KACST, SABIC, Saudi Aramco, and Caltech USA. He teaches polymer courses and supervises graduate theses, particularly in polyolefin catalysts and related chemistry and engineering. He chaired the organizing committee of an international materials science conference in 2022. He recently received nomination for the international *Premier Residency Special Talent Award* from Research Development Innovation Agency (RDIA) and King Abdulaziz City for Science & Technology (KACST), Saudi Arabia.

SULFUR-POISONING ON Rh NANOPARTICLE BUT SULFUR-PROMOTION ON SINGLE-Rh₁-SITE FOR CARBONYLATION

Siquan Feng, Jiali Mu, Qiao Yuan, Xingju Li, Yutong Cai, Xiangen Song, Jingwei Li and Yunjie Ding

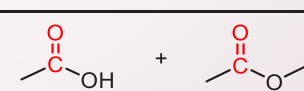
Chinese Academy of Science, China

Abstract:

Sulfur poisoning is a severe problem for most noble metal nanoparticle (NP) catalysts, and ppm or ppb levels of sulfur species could result in dramatic activity reduction or even irreversible deactivation. Developing catalysts with high sulfur tolerance is crucial, yet challenging. A heterogeneous single-site catalyst is promising to solve this problem.

Herein, a role reversal of sulfur from poison to resistant reagent or further promoter is presented for an Rh-based catalyst from supported Rh nanoparticle (NP) (Rh/AC) to its single-Rh₁-site (Rh₁/AC) in the reactions of methanol carbonylation, ethylene/acetylene hydrocarboxylation and olefins hydroformylation with a feed containing 1000 ppm H₂S. The Rh/AC was easily poisoned while the Rh₁/AC exhibited excellent sulfur-resistance activity. Detailed investigation indicated that H₂S could be rapidly transformed into catalyst-friendly CH₃SCH₃ and CH₃SH ligands on the single-Rh₁-site in the presence of CH₃I and/or CH₃OH, promoting acetyl production with a lower reaction energy barrier. Meanwhile, strong adsorption of sulfur species on Rh/AC formed an isolated Rh-S layer, blocking the adsorption of reactants.

Conditions: S-feed: S content 1000 ppm H₂S, Rh content was 1.0 wt.% for Rh/AC and Rh₁/AC. ^a 0.2g Rh/AC and 0.1g Rh₁/AC; 3.0 MPa CO, CH₃OH (218.75 mmol), CH₃I (20.98 mmol) for Rh₁/AC and 3.73mmol for Rh/AC, ultra-pure water (277.8 mmol), 433 K, 20 min in a zirconium autoclave reactor. ^b 0.22 g catalyst, acetic acid (100 mmol), CH₃I (2.77 mmol) and ultra-pure water (30 mmol), 0.2 MPa ethylene, 1.0 MPa normal CO or CO containing 1000 ppm H₂S, 453 K, zirconium autoclave reactor, 1h for Rh/AC, 3h for Rh₁/AC. ^c 0.3g catalysts, acetylene (4 mmol), CH₃I (8 mmol) and ultrapure water (500 mmol), 2.5 MPa normal CO or CO containing 1000 ppm H₂S, 453 K, zirconium autoclave reactor, 1.5 h for Rh/AC, 5 h for Rh₁/AC.

No	Catalysts	Conditions	Yield of products (%)	mole _{acetyl} /mole _{Rh} /h
		$\text{CH}_3\text{OH} + \text{CO} \xrightarrow{\text{Catalyst}}$ 		
1	Rh/AC ^a	Normal feed	10.2	163*
		S-feed	2.5 ↓	40* ↓
	Rh ₁ /AC ^a	Normal feed	70.2	2016
		S-feed	72.7 ↑	2477 ↑

		$\text{C}_2\text{H}_2 + \text{CO} + \text{H}_2\text{O} \xrightarrow{\text{Catalyst}} \text{C}_2\text{H}_3\text{COOH}$		
2	Rh/AC ^b	Normal feed	6.5	64.9
		S-feed	0.3 ↓	3.2 ↓
	Rh ₁ /AC ^b	Normal feed	39.2	136.2
		S-feed	68.8 ↑	215.2 ↑
		$\text{C}_3\text{H}_2 + \text{CO} + \text{H}_2\text{O} \xrightarrow{\text{Catalyst}} \text{C}_3\text{H}_3\text{COOH} + \text{C}_2\text{H}_3\text{COOH}$		
3	Rh/AC ^c	Normal feed	19.6	15.1
		S-feed	8.8 ↓	6.9 ↓
	Rh ₁ /AC ^c	Normal feed	37.7	9.4
		S-feed	56.7 ↑	14.2 ↑

Table 1. Effect of H₂S on the catalytic activity of Rh NP (Rh/AC) and single-site (Rh₁/AC) catalyst.

Biography

Siquan Feng received a Ph. D degree at the University of Chinese Academy of Science in Industrial Catalysis in 2019 and obtained the associate professor position at the Dalian Institute of Chemical Physicals, Chinese Academy of Science. He made many interesting works in the field of metal catalysis for the reactions of carbonylation. For example, the in-situ preparation of single-metal-site catalyst from the atomic dispersion of metal nanoparticles or ionic bonding or coordinate bonding into support of metal ion on the N/O/P site of organic porous polymer. The structure-activity of single-metal-site catalysts for methanol carbonylation and ethylene hydroformylation was addressed. The evolution of a single-Rh₁-site catalyst with the coordinate ligands during the reaction was disclosed. The relationship of single-metal-site catalysis between homogeneous and heterogeneous was also investigated. More interestingly, the sulfur-related structure-activity difference between the nanoparticle and single-metal-site catalyst for carbonylation was emphatically considered.

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NANOCATALYSIS FOR HYDROGEN GENERATION

Tokeer Ahmad

Jamia Millia Islamia, India

Abstract:

Multifunctional nanostructures as nanocatalysts find the possibility for their applications in water splitting processes for hydrogen generation as a renewable source of green energy. The studies of some multifunctional nanoparticles by chemical synthesis reveal the formation of monophasic nanostructures with fairly uniform distribution of nearly spherical particles, high specific surface area and visible optical band gap. Photocatalytic generation of hydrogen in water splitting process by using as-prepared nanoparticles has also been studied under the visible light irradiations which showed a significant H₂ evolution reaction rate. The development of nanostructured catalysts has also been preferred to carry out the heterogeneous catalytic organic transformations because of greater number of surface-active sites for catalytic processes, high catalyst recovery rate, especially their environment friendly nature and their ease of synthesis. Besides the advances in nanocatalysis, certain challenges including not well-defined morphologies due to loss of control over it and loss of catalytic activity during operation need to be addressed.

Biography

Tokeer Ahmad did his masters (chemistry) from IIT Roorkee and Ph.D. from IIT Delhi. Presently, he is full Professor at Jamia Millia Islamia, New Delhi. Prof. Ahmad has supervised 10 PhD's, 74 postgraduates, 9 research projects, published 132 research papers and two books with research citation of 4640, h-index of 41 and i10-index of 90. Prof. Ahmad is active reviewer of 112 journals, delivered 111 Invited talks and presented 124 conference papers. Prof. Ahmad has received DST-DFG award, ISCAS Medal, Inspired Teacher's President Award, Distinguished Scientist Award and elected as Member of National Academy of Sciences India. Prof. Ahmad has been figured in World Top 2% Scientists by Stanford University, USA and has also been conferred the prestigious Maulana Abul Kalam Azad Excellence Award of Education for the outstanding contribution in the field of education.



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PRODUCTION OF PURE HYDROGEN FROM NATURAL GAS CRACKING USING TITANIUM DIOXIDE SUPPORTED BIMETALLIC CATALYSTS

Wasim Ullah Khan, Hassan Alasiri, Ahmed Al Shoaibi, Srinivasakannan Chandrasekar and Mohammad Mozahar Hossain

King Fahd University of Petroleum & Minerals, Saudi Arabia

Abstract:

Despite the fact that fossil fuel-based energy sources still share a major portion of current energy demands, the combustion of these non-renewable energy sources leads to severe global environmental ramifications. In contrast, hydrogen, an alternative potential future fuel, upon combustion, produce environmentally friendly water, and hence, can replace existing non-renewable energy sources. Therefore, the scientific community has focused on the production of pure hydrogen in recent years. In this context, natural gas (methane) cracking and/or decomposition facilitates the facile process for pure hydrogen production along with valuable byproducts in the form of carbon nanomaterials with zero carbon footprint. In this work, we have synthesized nickel and cobalt-based bimetallic catalysts supported on titanium dioxide and evaluated their performance during methane decomposition reaction. The nickel-to-cobalt ratio was fixed as one and total metal loading varied between 20 to 60 wt%. The characterization of as-synthesized catalysts such as porosity and surface area analysis, X-ray diffraction (XRD) and temperature-programmed reduction (TPR) indicated that specific surface area and pore volume increased with an increase in metal amount until metal amount reached 50 wt% above which both specific surface area and pore volume decreased. However, TPR showed a linear increase in hydrogen uptake with increase in metal loading. The catalysts with higher amounts of metal (> 50 wt%) showed relatively weaker metal-support interaction and enhanced reducibility. XRD data indicated the existence of oxides of nickel and cobalt with anatase phase of titanium dioxide, however, no peaks of metal-titanate were found. The activity results demonstrated that the catalyst with 50 wt% metal loading remained the optimal performing catalyst with respect to methane conversion and carbon yield. The post-reaction characterization using thermogravimetric analysis and transition electron microscope demonstrated the formation of carbon nanotubes. The carbon growth mechanism was also discussed.

Biography

Wasim Ullah Khan received his BE in Chemical Engineering from the University of Engineering and Technology Lahore in 2008. Later, he joined the fertilizer industry where he worked in urea production for one year. He obtained his MS degree in Chemical Engineering from King Saud University Riyadh, Saudi Arabia, in 2015. He, then moved to New Zealand, to continue his doctoral degree, under the supervision of Dr. Alex Yip in the Energy and Environmental Catalysis Group at the University of Canterbury, New Zealand. He is currently serving as Assistant Professor (Research) at Interdisciplinary Research Center for Refining & Advanced Chemicals, Research Institute, King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia where his research focuses on the synthesis, characterization, and catalytic properties of bimetallic catalysts for hydrogen production from ammonia as well as natural gas decomposition along with the design and synthesis of transition metal-based catalyst for in-situ copolymerization of ethylene with polar monomer.

EFFECT OF A 6 WEEK PRESEASON TRAINING PROGRAM ON SALIVARY BIOMARKERS IN ELITE BASKETBALL ATHLETES

Mexis D, Nomikos T and Kostopoulos N

University of Athens, Greece

Abstract:

Aim: This study aimed to evaluate the effects of a 6-week pre-season training program on salivary biomarkers (free testosterone, cortisol, TBARS - thiobarbituric acid reactive substances), in elite male basketball players of Greek A2 National Division.

Material and Methods: The sample consisted of N=10 athletes (2 centers, 4 forwards, 4 guards) all from the same team, age=25.1 years, height=1.95cm, weight=91.7kg and body fat percentage=15.4%. The main weekly training schedule of the team included 6 basketball technical and tactical training units (TU) of 90' each, for the whole 6 weeks of the pre-season period. The intervention fitness protocol was added to the basic team training schedule, and each added fitness TU during the pre-season period lasted for 45'. More specifically, the intervention protocol consisted of 3 TU during the first week (2 strength TU – 1 conditioning TU), 4 TU during the second week (2 strength TU – 2 conditioning TU), 5 TU during the third week (3 strength TU – 2 conditioning TU), 5 TU during the fourth week (2 strength TU – 3 conditioning TU), 4 TU during the fifth week (2 strength TU – 2 conditioning TU) and 3 TU during the sixth and final week (1 strength TU – 2 conditioning TU). 7 saliva samples were collected from each player for the assessment of free testosterone, cortisol and TBARS. The biochemical measurements were carried out 7 times, before the beginning of the pre-season period, and after each week of the 6-week pre-season training period.

Results: The results showed no significant differences in free testosterone levels during the 6 week period. On the other hand, cortisol levels were significantly elevated after the 4th week compared to the 1st week (1st: 22.12 ± 9.92 , 4th: 37.71 ± 9.79 , $p=0.003$), and after the 3rd, 4th, 5th and 6th week compared to the 2nd week (2nd: 18.91 ± 8.7 , 3rd: 32.17 ± 14.14 , $p=0.047$), (2nd: 18.91 ± 8.7 , 4th: 37.71 ± 9.79 , $p<0.001$), (2nd: 18.91 ± 8.7 , 5th: 31.42 ± 9.49 , $p=0.02$), (2nd: 18.91 ± 8.7 , 6th: 29.92 ± 12.32 , $p=0.026$). Similarly, TBARS were significantly higher after the 4th week compared to the 3rd, 2nd, 1st, and to the first measurement before the preseason (pre: 1.8 ± 0.54 , 4th: 2.81 ± 0.71 , $p=0.007$), (1st: 1.72 ± 0.45 , 4th: 2.81 ± 0.71 , $p=0.001$), (2nd: 1.81 ± 0.45 , 4th: 2.81 ± 0.71 , $p=0.003$), (3rd: 2.17 ± 0.49 , 4th: 2.81 ± 0.71 , $p=0.047$). Finally, after the 2 last weeks we demonstrated some significant decreases in TBARS levels (3rd: 2.17 ± 0.49 , 6th: 1.53 ± 0.41 , $p=0.029$), (4th: 2.81 ± 0.71 , 5th: 2.1 ± 0.48 , $p=0.034$), (4th: 2.81 ± 0.71 , 6th: 1.53 ± 0.41 , $p=0.003$), (5th: 2.1 ± 0.48 , 6th: 1.53 ± 0.41 , $p=0.035$).

Conclusion: The pre-season training period in elite basketball can increase the levels of stress, as it is expressed through the cortisol hormone and the TBARS. Also, it has been noticed that at the end of the preseason period when the training schedule was lighter, there was a significant decrease in TBARS levels. Whether these alterations are useful for the adjustment of these athletes to the heavier physical demands of the regular basketball season or may diminish their performance requires further investigation.

Biography

Mexis Dimitrios is 4th year PhD Candidate and his area of expertise is the analysis of biomarkers that are related to muscle damage and inflammation, oxidative stress, metabolism and sports performance. He's been evolved in educating university students, studying and building his experience on this particular research area for almost a decade, and he is very passionate on creating a model that will help athletes to maximize their performance and diminish the risk of injuries.

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FREE-METAL CATALYST OF LAYERED DOUBLE HYDROXIDE/PET POLYMER FOR EFFICIENT THERMOMECHANICAL AND BARRIERS

Basharat Hussain

Chung Yuan Christian University, Taiwan

Abstract:

The unique thermomechanical and barrier properties of poly (ethylene terephthalate) PET make it widely used in various industries. However, PET causes major environmental problems globally due to present of metal-catalyst (antimony) in poly (ethylene terephthalate) (PET). In view of the fact that PET is almost impossible to replace with another material, an efficient approach for developing a light-metal catalyst for poly (ethylene terephthalate) (PET) that fulfills the demanding requirement of effective thermomechanical properties without antimony, cobalt, or another heavy metal. It is generally 95% of antimony (Sb) compounds that are used in the commercial synthesis of PET worldwide. There is no doubt that Sb is an extremely toxic trace element for mammals, and that it interferes with the development of embryos and fetuses, as well as being carcinogenic. Herein, a new kind of efficient light-metal catalyst layered double hydroxide (LDH) was developed through the calcium dodecylbenzene sulphonate Ablusol and n-Butyl alcohol surfactant commercial named Ablusol DBS-70NBA as organic surfactant. However, Ablusol DBS-70NBA anion intercalated LDH (LDH-NBA) was synthesized by hydrothermal method to enhanced the catalytic behaviors and compatibility of polymer with LDH. The efficiency of LDH-NBA comes from the intercalation of NBA, which has strong ability to compatible with PET chain through increment of LDH gallery, this will facilitate oligomer (polymer chain) to enter into LDH-NBA layers, during polymerization of the polymer matrix. Its structure was confirmed by X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy. The structural and dispersion morphologies of PET-LDH nanocomposites were investigated by field emission scanning electron microscope (FESEM) and transmission electron microscope TEM, X-ray diffraction (XRD), respectively. In these results, they were able to observe exfoliated dispersion of the LHD-NBA nanocomposite in PET polymer matrix, as a consequence the thermomechanical property of PET-LDH-NBA nanocomposites were enhanced by exfoliated micro-structure of LDH-NBA nanolayers. Additionally, during isothermal crystallization, in order to elucidate the effect of exfoliated nanolayers played a key role as nucleating agents, as confirmed by differential scanning calorimeters (DSC). Since nanocomposites have an increased nucleation site, they might crystallize more easily, which leads to altered the free metal (antimony) catalytic behavior of LDH-NBA as well as their thermomechanical properties and barrier.

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Biography

Basharat Hussain, a Ph.D. researcher under the supervision of Dr. Professor Tsung-Yen Tsai in the department of chemistry university of Chung Yuan Christian, Republic of Taiwan, since 2018. In my life, I have given myself a vision comprising several goals, some relating to my personal life and some to my life in the profession, which I do my best to accomplish. These goals are designed to make the most of the qualities I have found in me. One of such qualities is investigating the problems deeper and turning them into opportunities. My motivation was always towards chemistry. After graduation, I found that though I had learned a lot, I needed to know more about chemistry, so I did my master's in physical chemistry. However, the thirst is still there to go more in-depth, investigate deeper, design simple solutions to more complex problems, and invent. If you look into my career, I have always looked for entrepreneurial opportunities. I aim to work as a researcher/teacher and convert my research into sellable ideas, win funds, create company growth and sell to return to the innovation with a proud earning. That is where I want to see myself in the future. At this career stage, I learned how to research and dig deeper into the problems during my Ph.D. In this last four-year tenure, I have been working on polymer clay nanocomposites. The main focus of my research is to design a novel catalyst for poly (ethylene terephthalate) (PET) polymer application in packing materials and fibers without affecting its thermomechanical and barrier properties. Traditionally PET polymer was synthesized by using antimony "Sb" as a catalyst which is considered toxic and carcinogenic, so I designed new catalysts by using organic surfactants as a modifier, one of which I discussed in the abstract. In the future, I will try to make PET Bio-Degradable. It's a really big challenge for the researcher, however, it might be possible by mixing the different ratios of polylactic acid (PLA).

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WASTE-BASED NANOCATALYSTS FOR BIOFUEL (BIODIESEL) PRODUCTION

Tadios Tesfaye Mamo

Taiwan University, Taipei, Taiwan

Abstract:

In the current world, more than 65% of energy comes from fossil fuel, a non-renewable form of energy source. However, fossil fuel-based energy sources emit massive GHG during mining, processing, and usage. Hence, The deterioration of fossil fuel resources and its negative impact on the Globe Environment encourage researchers to find alternative and renewable forms of energy sources. Biodiesel is one of the most promising alternative energy source to replace fossil fuels. Unlike the fossile fuel, it needs high investment and processing costs. To foster market competitiveness for Biodiesel, it is necessary to produce Biodiesel from economically viable and environmentally sound feedstocks.

In Many countries, waste disposal from our daile meal is another environmental problem, especially in a country that does not have proper waste management. Furthermore, the productivity and purity of the Biodiesel depend on the catalyst we used. This study paper discusses the preparation of waste-based nanocatalysts with detailed characterizations, including XRD, SEM-EDS, and FTIR, to identify the catalyst properties and its activity through Tansesterfication Process.

Another bootle nack in the commercialization of Biodiesel is the feedstock price. This work uses waste feedstock, i.e., Waste cooking oil and Freshwater Microalgal oil, with waste-based nanocatalyst to produce Biodiesel. The Physico-chemical property of the Biodiesel has been characterized based on ASTM D6751 test method, and the B100 quality of the Biodiesel is in good agreement with the standards set.

Biography

Tadios Tesfaye is a Ph.D. Scholar at Academia Sinica, Taiwan, since 2020 under NANO science and technology institute. He got his masters in 2018 From Addis Ababa University with Environmental Science specialization in Energy and Climate Science. His research works and interest focus on synthesizing nanomaterials and composites for Biofuel Production and CO₂ reduction application. He published research articles in high-impact factor SCI(E) journals and also serve as a reviewer in different Journals.

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CHLOROALUMINATE $[\text{HN}_{222}][\text{Al}_2\text{Cl}_7]$ IONIC LIQUID IMMOBILIZED ON THE COPPER (II) OXIDE NANOPARTICLES $\{\text{CuO}[\text{HN}_{222}][\text{Al}_2\text{Cl}_7]\}$ USED IN CASE STUDY OF Chan-Evans-Lam COUPLING APPROACH

Meena Nemiwal, Parveen Kumar, Vijesh Tomar and Akta Soni

Malaviya National Institute of Technology, India

Abstract:

Medicinal chemistry and synthetic organic chemistry rely primarily on C-N bonds for their structures. The Chan-Lam reaction is one of the most effective and straightforward approaches for fabricating C-N bonds due to the copper catalyst involved. The current research reveals the most sophisticated Chan-Lam coupling process in which the N-arylation between aniline and phenylboronic acid take place exclusively in the presence of $\text{CuO}[\text{HN}_{222}][\text{Al}_2\text{Cl}_7]$ nanocatalyst under solvent-free, base-free condition at room temperature. This practical approach produced the products with good to excellent yields in acceptable reaction time (3 h). The nanocatalyst was characterized by Brunauer-Emmett-Teller (BET), Energy-dispersive X-ray spectroscopy (EDS), Fourier-transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Powder X-ray diffraction (P-XRD), and X-ray photoelectron spectroscopy (XPS). Additional eco-friendly aspects of this novel nanocatalyst include strong catalytic activity, ease of recovery of nanocatalyst from the reaction mixture via filtration, and reusability five times without significant performance loss.

Biography

Meena Nemiwal is working as Assistant Professor in Department of Chemistry, Malaviya National Institute of Technology, Jaipur India. She has done her Ph.D degree in 2002. Dr. Nemiwal has explored synthesis and properties of biobased nanomaterials extensively. She has several research papers published in the respective area. Keeping in view the importance of the proposed research field, she intends to exploit eco-friendly nanomaterials for the efficient synthetic processes. As of now she has approx. 56 research/review papers/ book chapters published in the field of nanomaterials and organic transformations and to establish herself in thematic field of research in the leading peer-reviewed journal like International Journal of Hydrogen Energy (Elsevier), Science of Total Environment (Elsevier), Inorganic Chemistry Communications (Elsevier), Mini-reviews in Organic Chemistry (Bentham Science), Tetrahedron (Elsevier), Synthetic Communications (Tylor and francic), Results in Chemistry(Elsevier) and Monatshefte für Chemie - Chemical Monthly (Springer). She has total citations till date 453, H-index-12, i10-15 and impact factor 82.05. Three (03) students are persuing Ph.D under her supervision and five (05) M.Sc. dissertations have been completed under her supervision. She has broad knowledge on the development of novel nanocatalysts for remediation of wastewater by photocatalytic dye degradation and metal ion sensing removal.

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POTENTIAL OF GREEN CHEMISTRY IN SMART CITIES' RENEWABLE ENERGY

Daria Nekhorosheva

National Research University Higher School of Economics, Russia

Abstract:

Background: Cities are responsible for 67%-76% of world's energy consumption and produce 71%-76% of energy related hazardous emissions. To meet the goals of Paris Climate Agreement and to follow NET Zero 2050 IEA roadmap, cities should define targets for RES and reach them by increasing the share of RES, including solar PV and biomass in energy balances.

Objective: To forecast the usage of green chemistry in smart cities.

Methods: Data were drawn from Deloitte Smart city rating, World bank and other official sources including official web-sites of the cities, which elicited information on the share of RES in the city, city population, GDP per capita, country investment in RES, position of the city in the ranking of smart cities and level of income in the country. A sample of 25 cities was selected. Data were analyzed by cluster analysis. And forecasts were made with mathematical methods.

Results: There were twenty-five cities analyzed. Three clusters of cities were formed, in which share of RES can reach 19.4%, 26.1%, 35.5% depending on the cluster. The results of this study showed that the share of renewable energy sources in fifteen cities has a potential to grow. Average growth of share of RES among cities is accounted by 14.4%. As the share of solar energy and biomass in RES energy production in the world is around 12.8% and 70% respectively, the potential contribution into energy production in cities of green chemistry is counted for 12.64%, where shares of solar energy and biomass are 1.84% and 10.8% respectively.

Conclusion: There is a necessity to reorganize cities' energy system through including additional capacity of RES to meet global aims. Overall contribution of green chemistry to the growth of RES can reach 12.64% in analyzed fifteen cities with open potential. This won't be reached until governments and cities' authorities introduce conditions and support for effective changes.

Biography

Daria Nekhorosheva has her expertise in evaluation and interest in improving energy sector worldwide due to bad condition of the environment and need to reduce emissions, in accordance with the Paris Climate Agreement (2015) and NET Zero 2050 scenario. Daria's analysis and results show opportunities for the growth of green energy and chemistry in smart cities. Scientific research at the intersection of sciences shows the possibilities for the development of the energy sector and green chemistry in particular. She has made this research after years of experience in research and evaluation in economic field and energy sector.

RETROALDOL CLEAVAGE OVER LAYER DOUBLE HYDROXIDES: EFFECT OF METAL COMPONENTS ON SELECTIVITY AND ACTIVITY

Eleonora Butenko and Alexey Kapustin

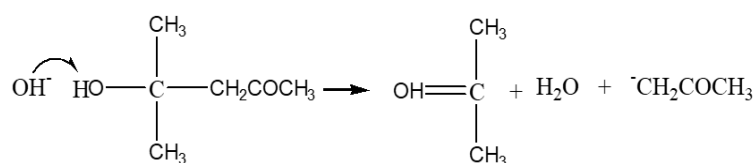
Azov Sea State Technical University, Ukraine

Abstract:

Retroaldol reactions take place in the presence of the base. One of these reactions is the transformation of diacetone alcohol to acetone.

Layer double hydroxides (LDHs) based on the hydrotalcite structure ($Mg_6Al_2(OH)_{16}CO_3 \cdot 4H_2O$) have been synthesized by coprecipitation with different Mg:Al ratios. The structure, and base properties have been studied. The base catalytic activity has been measured for the retroaldol cleavage. Activity data has been correlated with sample characteristics to gain insight into the active sites and mode of action of these catalysts. Selectivity data has been correlated with structure of these catalysts.

We have studied the retroaldol cleavage of diacetone alcohol in the presence of LDHs. The formation of acetone proceeds in the organic phase as a result of the interaction of the hydroxide ion with diacetone alcohol, which greatly speeds up the reaction rate:



We propose a mechanism for the retroaldol cleavage of diacetone alcohol in the presence of solid base, explaining the optimum way of forming acetone by filling the surface of the base with the diacetone alcohol and acetone anions.

The reaction order for diacetone alcohol in formation of acetone in the presence of solid NaOH is first. The reactions rate are dependence on the basicity of LDHs.

The by-products of reaction are mesityl oxide, phorone and i-phorone, because of flowing of aldol condensation of acetone. Selectivity of formation of by-products is related to the structure of LDHs.

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ENVIRONMENTAL FRIENDLY PLASTIC WASTE MANAGEMENT

Ravichandran

Lovely Professional University, India

Abstract:

Accumulation of plastic products in the Environment that adversely affects wildlife, habitat of humans is a major concern for the government at present. As plastic is non-biodegradable in nature, it remain in environment for several years. As a result it is responsible for causing land, air and water pollution. Plastic pollution has been constantly damaging our sustainable environment. The production of plastic is increasing since 1950, 8.3 billion tons of plastic has been produced, which is likely to be double by 2050. The burning of plastic waste increase the risk of heart disease, damages the nervous system, respiratory ailments such as asthma and cause nausea or headaches. Hence, a sustainable step towards tomorrow's greener and healthier environment needs immediate attention of the environmental scientists. Most of the environmental tools of plastics like cell phones, computers, helmets and hospital bags have molded society in many ways that make life both easier and safer. Plastic produced every year is used to make for single use, disposable packaging items or products when they are thrown out which damage the green environment. It is due to lack of self-discipline and not worrying about future generations, selfish attitude and consumerist human has damaged the environment. It is the responsibility of educational institutions to sensitize and create public awareness. In addition to creating public awareness on the importance of a clean and healthy environment, plastic recycling facilities must be recommended. This invited talk will help the society to reduce their exposures to plastics and ensure the increase of healthy society with clean environment for the next future generations.

Biography

S. Ravichandran is currently working as Professor in Department of Chemistry at Lovely Professional University, Jalandhar, Punjab (INDIA). He completed his Ph.D. in 2006 from Madurai Kamaraj University, Madurai (Tamilnadu) and M.Sc. from Pondicherry University, Pondicherry. He has qualified in GATE with a score of 95 percentile conducted by Ministry of Human Research and Development in the year 1998. He has 17 years of Research experience and published 135 International papers. He has published 7 Textbooks and received Bharat Shiksha and Life Time Education Excellence National awards from Global society in New Delhi. His area of research work are: Synthesis of Mannich and Schiff bases with metal ions like Cu(II), Co(II), Ni(II) and Zn (II). Structural characterization using spectroscopic techniques like UV-Vis., IR, ¹H NMR, CV, Chromatography and EPR. His current interest is to focus on the development of novel greener methodology for a Sustainable Development.

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March 20-21, 2023 | Rome, Italy



SYNTHESIS AND CHARACTERIZATIONS OF MoS_2/WO_3 HETERO-STRUCTURES FOR EFFICIENT PHOTOCATALYTIC EFFICIENCY

Faryal Idrees

The University of the Punjab, Pakistan

Abstract:

A novel hydrothermal ex situ synthesis was adopted to synthesize MoS_2/WO_3 heterostructures using two different molar ratios of 1:1 and 1:4. The "bottom-up" assembly was successfully developed to synthesize spherical and flaky-shaped heterostructures. Their structural, morphological, compositional, and bandgap characterizations were investigated through XRD, EDX, SEM, UV-Visible spectroscopy, and FTIR analysis. These analyses help to understand the agglomerated heterostructures of MoS_2/WO_3 for their possible photocatalytic application. Therefore, prepared heterostructures were tested for RhB photodegradation using solar light irradiation. The % efficiency of MoS_2/WO_3 composites for 30 min irradiation of 1:1 was 91.41% and for 1:4 was 98.16%. Similarly, the % efficiency of 1:1 MoS_2/WO_3 heterostructures for 60 min exposure was 92.68%; for 1:4, it was observed as 98.56%; and for 90 min exposure, the % efficiency of 1:1 was 92.41%, and 98.48% was calculated for 1:4 composites. The photocatalytic efficiency was further verified by reusability experiments (three cycles), and the characterization results afterward indicated the ensemble of crystalline planes that were responsible for the high efficiency. Moreover, these heterostructures showed stability over three cycles, indicating their future applications for other photocatalytic applications.

Biography

Faryal Idrees has published 59 SCI papers/book chapters as author/coauthor in SCI journals with well-renowned publishers. Her impact factor is more than 300 with 48-i10-index, 30-h index. She provided her services as a reviewer to many International Journals. She has successfully guest edited two special issues of well-reputed journals. She has won two international grants and working on different research projects. Currently, she is working as Assistant Professor in the Department of Physics, University of the Punjab, Lahore. She completed her post-doctoral fellowship from Photocatalysis and Nanotechnology, Institute of Technical Chemistry, Gottfried Wilhelm Leibniz University of Hannover, Germany under Alexander-von-Humboldt-Stiftung, one of the prestigious award in Germany. She is among the 2% Pakistani females who have gotten this opportunity so far. She worked there as a senior scientist and developed a new synthesis route to attain high molecular hydrogen production (renewable energy resources). Moreover, bachelor and master students conducted their research under her supervision. She completed her PhD in July 2015 in materials physics and chemistry from Beijing Institute of Technology, China. She is awarded by Distinguished and Excellent Student awards consecutively two times in 2013 and 2014. In PhD, her research work focused on materials synthesis, optical properties, photocatalysis and energy storage/conversion devices. During PhD, she developed a photocatalytic degradation setup in her lab. One of her work, based on green energy materials for energy storage/conversion devices is highly appreciated in scientific society and reported by renowned blogs: science daily and physics organization. Other than these she has also participated in different international conferences, workshops and science forums. More particularly, she presented her work in Malaysia, Berlin, Frankfurt, Dresden and Russia (Saint Petersburg).

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Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



THE PHARMACOLOGICAL ACTIVITY OF TULSI (*Ocimum sanctum*)

Prerna Sharma

Guru Gobind Singh College of Pharmacy, India

Abstract:

In the present review, an attempt has been made to congregate the botanical, phytochemical, pharmacological and toxicological information on Tulsi (*Ocimum sanctum*, *Lamiaceae*). OS has been adored in almost all ancient ayurvedic texts for its extraordinary medicinal properties. It is pungent and bitter in taste and hot, light and dry in effect. Its seeds are considered to be cold in effect. The roots, leaves and seeds of Tulsi possess several medicinal properties such as stimulant, aromatic and antipyretic. This plant has been known to possess antibacterial activity, antianaphylactic activity, antihistaminic and mast cell stabilization activity, wound healing effect, radioprotective effect, antidiabetic effect, antioxidant activity, anti-carcinogenic properties, immunologic effects, contraceptive effect, anti genotoxic effect, neuroprotective effect, cardio-protective effect and other miscellaneous activities. This review help for the researchers as well as clinicians dealing with *O. sanctum* to know its proper usage as this herb is seemed to be highly valuable, possessing many pharmacological / medicinal properties.

Biography

Prerna Sharma is currently working as a associate professor in Guru Gobind Singh College of Pharmacy, Yamunanagar . She is 10.5 years teaching experience as associate professor and Training & Placement Officer and she is selected as panel expert for AICTE STTP Programme. Her field of specialization is Pharmacogonosy and She has completed his master in Pharmaceutical sciences (2012) honour with gold medalist / appreciation in RITS ,Sirsa, India and recently she is purusing his PhD from the Uttarakhand Techical University, Dehradun, India, Her field of expertise is standardization of herbal plants/ herbal formulation.Her research area includes pharmacognostical & phytochemical investigation of Indian medicinal plants, She has 20 research/review publication national/international journals of repute to her credit, 40 Copyrights, 2 Patents and deligated more than 30 National/international conferences /workshops. She is honored with young research scientist award by SPER and TIPPA in Thailand .She is also president in SPER women forum and life member of professional bodies like association of pharmaceutical teachers of India(APTI).

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



METAL-ORGANIC COORDINATION COMPOUNDS OF MANGANESE(II) CONTAINING TEREPHTHALATE, BIPYRIDINE, AND TERPYRIDINE LIGANDS: SYNTHESSES, CRYSTAL STRUCTURES, AND CATALYTIC OXIDATION PROPERTIES

Isaac Yissa Aaron, Tella AC, Aswathy TV, Prabu M, and Raja T

University of Ilorin, Nigeria

Abstract:

Two new metal-organic coordination compounds of manganese (II), $[\text{Mn}_3(\text{H}_2\text{bdc})_3(\text{bipy})_2]\cdot\text{DMF}$ (1) and $[\text{Mn}(\text{Tpy})(\text{NO}_3)_2(\text{H}_2\text{O})]$ (2), comprising of terephthalate, bipyridine, and terpyridine ligands have been synthesized and characterized by UV-Vis and IR spectroscopies, XPS, BET, SEM, elemental and single crystal X-ray diffraction analyses. Compound 1 presents a trinuclear polymeric framework of Mn(II) atoms, carboxylate (H_2BDC) and terminal chelating bipyridyl ligands as the main coordinating species; the chelating bipyridine ligand has an additional structural consequence which confines the propagation of Mn/ H_2BDC /Bipy linkages to one or two dimensional polymeric frameworks. Compound 2 on the hand, presents an heptahedral, comprising of one Mn(II) atom, polypyridyl ligand (2,2':6,2''-terpyridine), water and nitrate molecules which are coordinated lattice species. To our knowledge, compound 2 is the first example of an asymmetric polypyridyl derivative of Mn(II) obtained by room temperature synthesis. The crystals of compound 1 are triclinic, space group P-1; $a = 9.8393(6) \text{ \AA}$, $b = 15.6758(10) \text{ \AA}$, $c = 15.7880(10) \text{ \AA}$, $\alpha = 108.566(2)^\circ$, $\beta = 90.596(2)^\circ$, $\gamma = 90.340(2)^\circ$, $V = 2308.2(3) \text{ \AA}^3$ and $Z = 2$. Similarly, the crystals of compound 2 are triclinic, space group P-1; $a = 7.6914(6) \text{ \AA}$, $b = 9.9173(7) \text{ \AA}$, $c = 12.4110(9) \text{ \AA}$, $\alpha = 71.885(7)^\circ$, $\beta = 80.875(6)^\circ$, $\gamma = 72.251(6)^\circ$, $V = 854.81(11) \text{ \AA}^3$ and $Z = 2$. Compounds 1 and 2 are chemically stable and have been utilized as effective catalysts for the 'green synthesis of adipic acid' from cyclohexanone, using H_2O_2 as the main oxidizing agent.

Biography

Isaac Yissa Aaron has his expertise in chemical sciences, specifically preparation of polymeric materials for use in catalysis, adsorption (water purification), quantum dots and as sensor devices. His passion for humanity and finding new pathways for improving healthcare by providing pure drinkable water, and creating new improvements for carrying out catalytic reactions has afforded diverse opportunities to build his career in research, and teaching in both education and research institutions.

European Congress on

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



DISTAL FUNCTIONALIZATION VIA TRANSITION METAL CATALYSIS

Haibo Ge

Texas Tech University, USA

Abstract:

The ubiquitous presence of sp^3 C–H bonds in natural feedstock makes them inexpensive, easily accessible, and attractive synthons for the preparation of common and/or complex molecular frameworks in biologically active natural products, pharmaceuticals, agrochemicals, and materials. However, the inertness of these bonds due to the high bond dissociation energies and low polarity difference between the carbon and hydrogen atoms makes them challenging reaction partners. Moreover, the desired site-selectivity is often an issue in reactions with multiple analogous sp^3 C–H bonds. To overcome these problems, transition metal-catalyzed C–H functionalization has been developed with the assistance of various well-designed directing groups which can coordinate to a metal center to deliver it on a targeted C–H bond through an appropriate spatial arrangement, enabling C–H activation *via* the formation of a cyclometalated species. However, the requirement of often additional steps for the construction of the directing groups and their subsequent removal after the desired operation severely hampers the efficacy and compatibility of the reactions. A promising solution would be the utilization of a transient ligand which can bind to the substrate and coordinate to the metal center in a reversible fashion. In this way, the directing group is installed, sp^3 C–H functionalization occurs, and the directing group is then removed *in situ* without affecting the substrate function after the catalysis is finished. Overall, the whole process occurs in a single reaction pot. Herein, we are presenting our studies on transition metal-catalyzed transient directing group-enabled C–H functionalization reaction.

Biography

Haibo Ge received his PhD degree in Medicinal Chemistry from The University of Kansas in 2006, and then moved to The Scripps Research Institute for postdoctoral study. In 2009, he began his independent academic career at the Indiana University – Purdue University Indianapolis and relocated to Texas Tech University in 2020. Research by his group is mainly focused on the development of novel methods for carbon–carbon and carbon–heteroatom bond formation through transition metal catalyzed C–H functionalization. His Research interests are "Transition metal catalyzed cross coupling reactions". His no. of published articles and Journals information are more than 60 publications including Nature Chemistry, Journal of the American Chemistry Society, Chem, Angewandte Chemie International Edition, etc.

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Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



REVIEW OF RESEARCH TOPICS FOR SCALING-UP OF SONOCHEMICAL REACTORS (SONO-REACTORS)

Orlando Elguera Ysnaga

Universidade de São Paulo, Brazil

Abstract:

This study is aimed to review the topics of chemical engineering to take in consideration for the scaling-up of reactors, in order to perform processes based on the application of the sonochemistry at industrial level. Sonochemistry is an emergent technology, defined as chemistry made with ultrasound. The characteristic ultrasound frequencies are in the range of 1-10 MHz, and in particular for sonochemistry in the sub-range 16-100 KHz. Chemical effects of ultrasound exist when there are changes in the path-ways of reactions, yields and/or selectivities of the products due to the ultrasonic activation. At laboratory level, the sonochemistry has shown fantastic results, because it is based on the phenomenon of acoustic cavitation in liquids, thus, producing very high temperatures (some thousands of Kelvin degrees) and high pressures (some hundreds of atmospheres) during very short times (from tenths to hundreds of microseconds). Cavitation is the phenomenon with the most important effect for intensification of physical and chemical processing. Under these conditions, the yields of sonochemical reactions increase drastically, and their selectivities are improved, thus generating new mechanisms of reaction involving inorganic and organic syntheses. It is not easy to reproduce experimental results of quantification of sonochemical intensity, which is significant for the efficient scaling-up of sonochemical reactors (Sono reactors) for the progress of industrial applications of sonochemistry. This technology has application at industrial level for the treatment of waste-water and black-water. Sonochemistry can be considered as Green Chemistry, presenting the following advantages: low waste, low consumption of materials and energy with optimized use of non-renewable resources and use of renewable energies. Few studies were aimed about optimum design and scaling-up of sonochemical reactors. The implementation of sonochemistry at the industrial level will be feasible when the use of cavitation energy can be adequately controlled.

Biography

Orlando Elguera studied Chemical Engineering at the National University of Engineering (Lima-Peru) with Master's studies in Chemistry Sciences at the National University of Engineering (Lima-Peru), and with Doctorate of Science with Major in Analytical and Inorganic Chemistry at the University of São Paulo (São Paulo-Brazil). He performed as Analyst of the Laboratory of samples of Geochemical Exploration and Inorganic Compounds at SGS del Perú S.A.C (almost 5 years). He has experience in the following method of analysis: Atomic Absorption Spectrometry, Inductively Coupled Plasma Optical Emission- Mass Spectrometry and X-ray Fluorescence. He has published 9 research articles in journals.

European Congress on

Chemistry and Applied Sciences

International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



TYROSINASES IN WETLANDS: GLOBAL CONTRIBUTORS TO CLIMATE CHANGE!

Felix Panis and Annette Rompel

University of Vienna, Austria

Abstract:

Wetlands are globally distributed ecosystems characterized by permanent or seasonal waterlogging, leading to predominantly anoxic soils. While wetlands sequester CO₂ from the atmosphere *via* plant photosynthesis, they exhibit low rates of organic matter decomposition and have, therefore, accumulated vast organic carbon stores of 550×10^{15} g of carbon (which is equivalent to 73% of the atmospheric carbon pool) over the last millennia. Phenolic compounds are crucial for the inhibition of organic matter degradation in wetland soils, as they act as broad-scale inhibitors of hydrolytic enzymes. Tyrosinases (TYRs) are oxidoreductases capable of removing phenolic compounds in the presence of O₂ by oxidizing them to the corresponding quinones. Within recent decades, the biochemical properties of bacterial tyrosinases have been investigated in detail, while investigations focused on carbon fluxes in wetlands on a macroscopic level have remained a thriving yet separated research area so far. To straddle these two previously separated research areas a phylogenetically diverse set of 145 TYR-producing bacteria (covering seven phyla: Acidobacteria, Actinobacteria, Bacteroidetes, Firmicutes, Nitrospirae, Planctomycetes, and Proteobacteria) indigenous to a global continuum of wetland ecosystems ranging from arctic zones to the tropics and their corresponding TYR enzymes (including DNA sequences and amino acid sequences) has been identified. *Via* a literature review, it has been demonstrated that TYR activity is commonly observed at pH values characteristic for wetland ecosystems and towards phenolic compounds commonly encountered within wetlands (*p*-coumaric acid, gallic acid, protocatechuic acid, *p*-hydroxybenzoic acid, caffeic acid, catechin, and epicatechin). These findings have been supported by biochemical investigations of a recombinantly expressed TYR (SzTYR), which is produced by an organism indigenous to globally distributed wetlands (*Streptomyces* sp. ZL-24). Taken together, these results underline the important role of TYRs as key enzymes controlling carbon storage in wetland ecosystems.

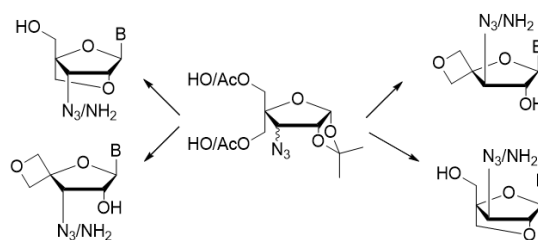
Biography

After successfully completing his master's studies in pharmacy, Felix Panis started his Ph.D. studies at the University of Vienna. During this time, he established a novel research area by straddling two previously separated fields, namely the biochemical investigations of tyrosinase enzymes and investigations focused on carbon fluxes in wetland ecosystems. This multidisciplinary work, located at the intersection between biochemistry and soil sciences, became the central theme of his Ph.D. studies and is currently being progressed during his postdoctoral research employment. The motivation for this interdisciplinary research approach stems from the firm belief of Felix Panis that, in the face of climate change, it is science that will decide the future course of the global climate crisis. Novel and innovative approaches, as they are currently being developed by Felix Panis, will offer tools and possibilities to analyze, predict, and mitigate the effects of global climate change by developing and improving strategies for the protection and restoration of wetland ecosystems.

BIOCATALYST MEDIATED SYNTHESIS OF MODIFIED NUCLEOSIDES**Rajesh Kumar***R.D.S. College (B.R.A. Bihar University), India***Abstract:**

Over two decades, a large number of nucleosides have been synthesized, which demonstrated potent antiviral and antitumour activities and have become corner stones of treatment for patients with cancer or viral infections. Oligonucleotide-based antisense strategies represent a unique paradigm for the treatment of a wide variety of human diseases. In order to discover new class of nucleoside derivatives with enhanced biological activities, the modifications in the sugar moiety have been attempted, which provide a remarkable level of control over nucleoside sugar puckering and its biological activity.

Herein, we report; (a) the selective biocatalytic acetylation studies on modified 3'-azido-4'-C-hydroxymethylated sugar derivatives with an aim to develop an efficient and easy method for the synthesis of ribo-azido/amino LNA monomers and xylo-azido/amino spiro-oxetano nucleosides and (b) the selective biocatalytic deacetylation studies on modified 3'-azido-4'-C-acetoxymethylated sugar derivatives with an aim to develop an efficient and easy method for the synthesis of ribo-azido/amino spiro-oxetano nucleosides and xylo-azido/amino LNA monomers.



B = Nucleo Bases (T, U, C & A)

Biography

Rajesh Kumar received his M.Sc. degree in Organic Chemistry in 2010 and Ph.D. in 2017 from the University of Delhi. During his Ph. D research work he worked as a Research Assistant in the University of Southern Denmark. After completing his Ph.D. he joined as an Assistant Professor at B.R.A. Bihar University, India. He has published 30 research papers in reputed national and international journals. His research interest lies in nucleic acid chemistry, biotransformation's, catalysis and heterocyclic chemistry.

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



EFFECT OF SECONDARY COMBUSTION ON THRUST REGULATION OF GAS GENERATOR CYCLE ROCKET ENGINE

Muhammad Umer Sohail, Sohaib Khan, Ihtzaz Qamar, Muzna Tariq and Raees Fida Swati

Institute of Space Technology, Pakistan

Abstract:

Thrust regulation is applied to maintain the performance of the liquid propellant rocket engine. The thrust level of a rocket engine can be readily controlled by adjusting the number of propellants introduced into the combustion chamber. In this study, a gas generator design is proposed in which thrust regulation is maintained by performing secondary combustion in the divergent section of the nozzle of a gas generator. Tangential and normal injection techniques have also been studied for better combustion analyses. A normal injection technique is used for the experiment and CFD results are validated with the experimental data. Chemical equilibrium analyses are also performed by minimizing Gibbs free energy with the steepest descent method augmented by the Nelder–Mead algorithm. These equilibrium calculations give the combustion species as obtained through the CFD results. Performance evaluation of the rocket engine, with and without secondary combustion in the gas generator, led to an increase of 42% thrust and 46.15% of specific impulse with secondary combustion in the gas generator.

Biography

Muhammad Umer Sohail (PhD Aerospace Engineering, MS Power Mechanical Engineering, MBA Executive, BS Mechanical Engineering) has repeated success guiding sizeable, cross functional engineering and product development teams with inculcation of knowledge, skills and application of experience to define novel solutions of aerodynamics and fluid flows. I have 12 years of academic and research experience. I have supervised number of undergraduate/graduate engineering students, research based industrial projects and participated many national level events. I am currently serving as an assistant professor in Aeronautics & Astronautics Engineering Department of Institute of Space Technology, Islamabad, Pakistan.

TRANSCRIPT EXPRESSION LEVEL ANALYSIS OF PHYTOENE SYNTHASE AND PHYTOENE DESATURASE ASSOCIATED WITH β -CAROTENE CONTENT AND GENETIC TRANSFORMABILITY IN BITTER MELON

Labode Stevenson Naitchede

Institute for Basic Sciences, Technology, and Innovation, Kenya

Abstract:

Bitter melon (*Momordica charantia* L.) is a widely cultivated food and medicinal plant native to the world's subtropics and tropics. Constraints affecting the cultivation of Bitter melon affect the productivity of β -carotene. Knowing the mechanism that controls the transcription of the β -carotene biosynthesis genes in bitter melon will be of great value in improving the yield of this important metabolite. The expressions of β -carotene biosynthetic genes such as Phytoene Desaturase (PDS) and Phytoene Synthase (PSY) were evaluated in bitter melon accessions 'GBK027049', 'NS1026', 'Mahy-ventura', '453B' and 'Sibuka532'. Transcript expression level analysis of PSY and PDS, and the amount of β -carotene in leaf, stem, and fruit, were determined using quantitative polymerase chain reaction and high-performance liquid chromatography (HPLC). Root transcript expression was used as a negative control for determining the relative fold change in other tissues. *Agrobacterium tumefaciens* strain EHA105 harboring a plasmid with the β glucuronidase (GUS) reporter gene was used to test the transformability of bitter melon leaf, and the resulting calli were assayed for GUS activity. The expression of PSY in the fruit (6 to 27-fold compared to the control) was higher than in the other organs for all accessions. This was also the case of PDS expression (10 to 29-fold compared to the control). Leaves had the highest β -carotene concentration (17.92-45.35 $\mu\text{g}\cdot\text{g}^{-1}$); there was no difference between stems (5.67-12.75 $\mu\text{g}\cdot\text{g}^{-1}$) and fruit (6.18-12.53 $\mu\text{g}\cdot\text{g}^{-1}$). The highest β -carotene content was in accessions 'GBK027049' (12.53-45.35 $\mu\text{g}\cdot\text{g}^{-1}$) and '453B' (6.18-32.09 $\mu\text{g}\cdot\text{g}^{-1}$). PSY and PDS expressions positively correlated with the amount of β -carotene in leaves, stems, and fruits. Bitter melon leaves, especially those of 'GBK027049' and '453B' accessions, are an alternative to alleviate the β -carotene deficiencies in the world. The leaf was successfully transformed by EHA105 harboring the reporter gene GUS with a transient expression frequency of 53.7%.

Biography

Labode Stevenson Naitchede has expertise in evaluation and passion in gene expression, tissue culture, and plant transformation to provide food security and well-being. He established the correlation between PSY and PDS expressions and β -carotene levels and developed a regeneration protocol in bitter melon, which contributed to breeding and conservation programs, industrial value addition, and trade of bitter melon. His model based on the transformation of medicinal plants is of great value in overcoming the deficiency of vitamin A in the world.

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International Conference on &

Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



NATIONAL FOOD CONTROL SYSTEM IN INDIA

Prem Kumar Jaiswal

Former Director of Labs, CAL, Govt. of India, Adviser Food Safety, India

Abstract:

National food control system in India has under-gone tremendous changes consequently upon formation of Food Safety and Standards Authority of India vide Food Safety Act 2006, its Rules 2011 and numerous Regulations. International trade of food amongst different countries have facilitated and increased many folds due to liberalisation of trade, uniformity in food standards, harmonisation of country standards with that of Codex Standards and mutual acceptance and recognition of standards and testing protocols/internationally accredited testing laboratories.

In the present communication, objectives, scope, key principles, components like food chain, frame work, policy setting of food control system., system design, implementation, monitoring and system review, strengthening food control system have been discussed.

The challenge for food regulator is to implement a food regulatory control system that delivers safe food to the public, enable customers to make informed of right choices and gain public confidence in food regulatory system.

Food safety is a shared responsibility among government, all parties involved in the food chain including primary production, handling, storage, processing, packaging, transportation, distribution and sale of food products, and consumers.

Consumers need to be made aware of the importance of food safety in protecting themselves against food safety hazards both in the choice and preparation of food. Demarcation of food control system between state and central regulator, role of private agencies in food control system, importance of self-compliance by FBO, training and awareness by state and central agencies should be focused with a view to have a strong food safety eco system in a country.

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March 20-21, 2023 | Rome, Italy



ARTIFICIAL INTELLIGENCE BASED MODELLING AND OPTIMIZATION OF CATALYST IN REAL INDUSTRIAL PLANT TO SIMULTANEOUSLY ENHANCE PROFIT AND REDUCE NEGATIVE ENVIRONMENTAL IMPACT

Sandip Kumar Lahiri and Somnath Chowdhury

National Institute of Technology, Durgapur, India

Abstract:

In order to measure their environmental impact and strike a delicate balance between profit and environmental impact, catalyst in commercial chemical plants can employ the new artificial intelligence-based modelling and optimization methods proposed in this work. In situations when creating phenomenological models for commercial catalyst is either challenging or time-consuming, this work demonstrates an artificial intelligence (AI) based genetic programming modelling methodology for commercial complex reactors using existing industry data. In the current study, a multi-objective hybrid genetic programming and metaheuristic optimization algorithm are employed to strike a delicate balance between financial success and environmental effect of commercial catalyst. A detailed case study of silver-based catalyst employed in the commercial ethylene oxide (EO) manufacturing process is used to demonstrate the usefulness of the suggested methodology. The suggested methodology creates the best process condition for EO reactor operation, which currently used in commercial plants to increase catalyst selectivity and revenue. This research also suggest how an explainable AI methodology can be effectively used to gain insights of actual catalyst performance in real plant and exploit that knowledge to increase profit. Additionally, the suggested methodology creates a platform for Pareto optimal solutions to acquire insights into the balance between profit and environmental impact. The plant management may find these insights to be very helpful in making decisions about the operations of the plant. The developed methodology made use of the most recent AI-based modelling and optimization techniques that were inspired by nature. It is generic and may be used to any other operating plant. This work also suggests how to build an online optimizer, and in the plant's ever changing dynamic environment, the best conditions can be maintained. For operating catalyst in commercial chemical plants, the suggested methodology strikes an overall balance between profit and environmental impact.

Biography

Sandip Kumar Lahiri is a professional Chemical Engineer with Doctorate degree (PhD) in Chemical Engineering. Over 50+ technical publications in leading international journals in chemical engineering covering subjects like modelling and simulation, artificial intelligence, process design, optimization, fault diagnosis, CFD etc. and he is the author of 3 books published by Wiley and Springer. US Patent holder "Online Fault Diagnosis in Chemical plant" Professional. He had Wide international exposure in petrochemical companies across globe. He is Working as a technical consultant in Europe (BASF, Germany, Sasol, Germany, Ineos, Belgium, BASF, Belgium,) Saudi Arabia (Sabic, Saudi Arabia), India (Reliance, India, IOCL, India), Thailand (PTT group, Thailand) etc. Over 28 years' experience in production, technical services and technology advisor of leading petrochemical industries across globe in leadership position. Currently works faculty in National Institute of Technology, Durgapur, India. Expertise in implementing Industry 4.0 application, APC (Advance process control), fault diagnosis system, debottlenecking study, energy optimization study in process plants across globe. He had listed in World Who's Who (2010,2012 and 2015 edition) as significant contributor & achiever in chemical industry

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Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



CHEMICAL PROCESS-CONTROL in line WITH 4 METHODS OF FIBER SPECTROSCOPY

Viacheslav Artyushenko

Art photonics GmbH, Germany

Abstract:

The latest fiber-optic techniques in spectral range from UV to mid-infrared will be reviewed for research and industrial applications. Fiber optic probes enable to run sampling-free remote process monitoring. Depending on the chemical process & media to be analyzed, fiber probes can be based on 4 different fiber types selected for the required spectral range and used for Transmission, Reflection, ATR-absorption, Raman & Fluorescence spectroscopies. Advanced fiber optic combi probes are capable to utilize two spectroscopic methods at the same time assembled in the same probe shaft - such as Mid-FTIR+Fluorescence, Raman+Near IR, Raman+Mid-FTIR and others. It improves selectivity and precision of the analysis for media content in process control.

Robust fiber probes are reliable in a variety of applications, including harsh environments, such as wide temperature range from -150°C to +250°C, high pressure up to 200 Bar or in vacuum, aggressive liquids or gases, electromagnetic fields, including microwave and hard radiation and vibrations.

In the case of complex samples, single spectroscopic technique may be not sufficient for reliable control and monitoring of the process. Such challenging analytical tasks may require an optical diagnostic where different spectroscopic methods are combined to achieve better accuracy. In this case, the capability of the combined methods to deliver complementary chemical information creates a synergy. Moreover, advanced fiber optic combi probes collect spectral information from the same spot. In addition, the process can be investigated in the laboratory using all kinds of spectroscopy techniques. Several examples of different fiber spectroscopy applications will be presented using different methods and their combinations. Based on the results, a customized sensor based on a few, but key informative spectral bands can be developed - with reduced size and cost.

Biography

Viacheslav Artyushenko was born in 1954 and got his PhD in physics of solid state in 1981 – focused on his pioneering development of unique technology of polycrystalline fibers for Mid IR-range: 3-18µm. His multiple publications and patents were devoted to specialty fiber optic technologies and their applications in laser surgery and diagnostics, in process-spectroscopy and fiber optic sensing. In 1998, he has founded art photonics GmbH in Berlin – one of the worldwide leading manufacturers of various fibers, cables, bundles and spectroscopy probes used in very broad spectral range 0.3-16µm for many industrial, medical, scientific and other applications. Dr. V. Artyushenko is member of EPIC, CPACT, SPIE, OSA, SAS, SPECTARIS, Optec-BB, Photonics-BB, GDCh-DECHEMA & CLIRSPEC.

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HETEROGENEOUS FENTON-LIKE PROCESS OVER STEEL SCALE WASTE FOR THE TREATMENT OF LANDFILL LEACHATE

Eleonora Aneggi

University of Udine, Italy

Abstract:

Sustainable industrial processes are essential for better economic growths and for the conservation of the environment. In this study we have employed steel scale waste (SSW), a by-products of steel production containing oxides in large quantity, as a heterogeneous Fenton-like catalyst for the treatment of landfill leachate to implement the concept of “sustainable circular economy”. Landfill leachate is a very complex liquid waste mainly consisting of refractory organics, heavy metals, ammoniacal nitrogen and chlorides. Biological treatment of landfill leachate is not effective and advanced oxidation processes (AOPs) are needed due to their ability to mineralize organics and to enhance the biodegradability of treated liquid wastes. This concept of employing solid waste (steel waste) for the treatment of liquid waste is very important for achieving the goals of sustainable growth and waste minimization. In this research we have investigated the catalytic ability of steel scale as a heterogeneous Fenton like catalyst for the treatment of a complex liquid waste such as leachate under variable conditions of steel scale dose, pH, temperature, and oxidant dose. At mild conditions SSW successfully removed about 75% of the recalcitrant organic loading from landfill leachate, resulting in a promising material for the treatment of heavily polluted wastewater streams. These findings appear extremely important from a circular economy perspective, because steel scale waste is produced in huge quantities and could be effectively used as a catalyst in a highly polluted liquid waste treatment process.



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Poster Presentation

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INVESTIGATING THE PERFORMANCE OF SPINEL MATERIALS MgX_2O_4 (X=Mn, Ni, Co) AS POTENTIAL CATHODES IN MAGNESIUM-ION BATTERIES

Ali Zeinodiny, Soheila Javadian and Nima Dalir

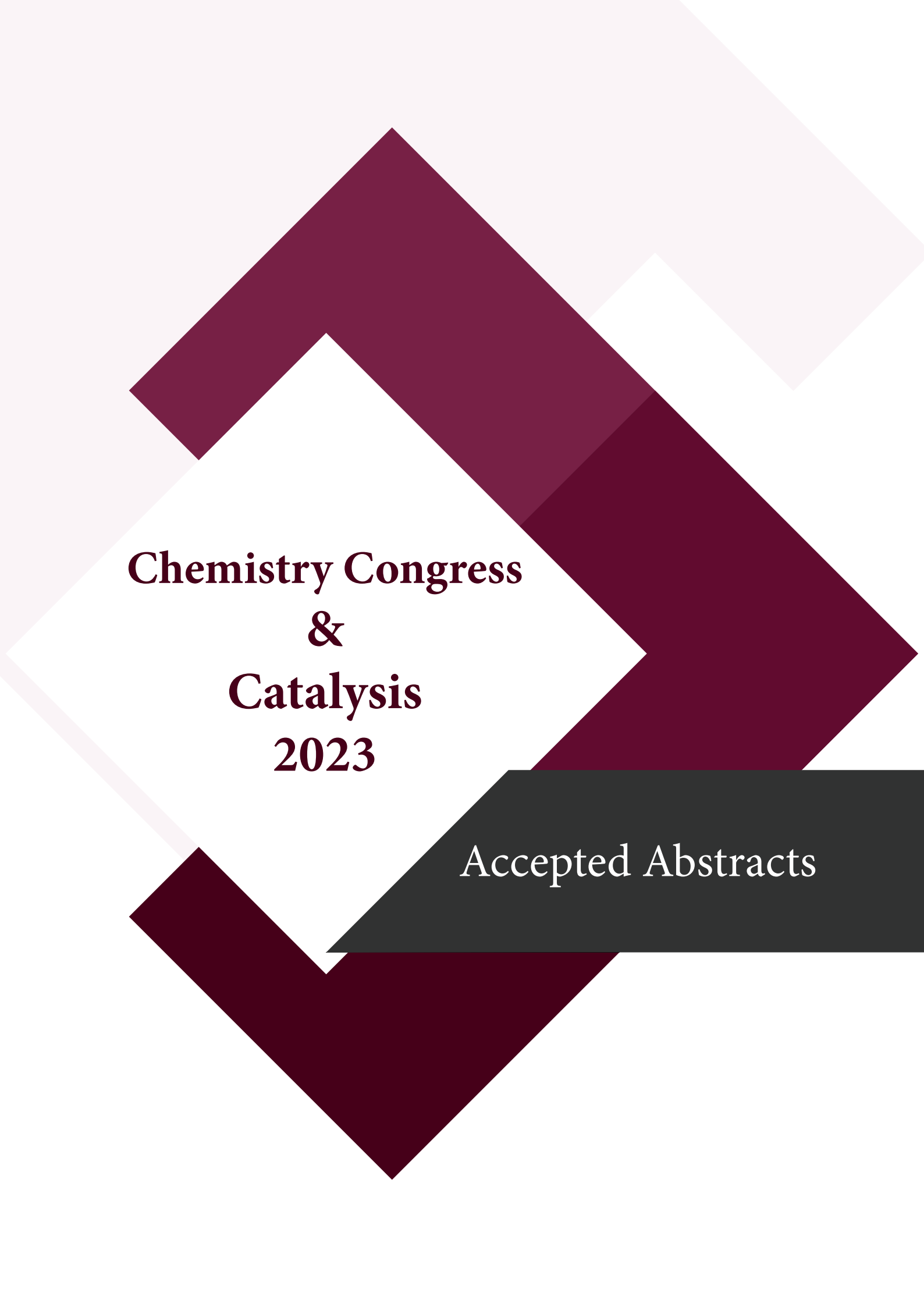
Tarbiat Modares University, Iran

Abstract:

Magnesium-ion batteries have been researched and interested by scientists as a new technology for the post-lithium era. But the cathodes used in them are considered as a problem in their commercialization. There are several important parameters in choosing the right cathode, which can be mentioned as high capacity and proper stability in long charge and discharge cycles. In this research, different types of spinel cathodes have been studied and their performance and stability have been evaluated. These cathodes were synthesized by a facile one-step self-template method using glycerine as template. Charge and discharge test for spinel materials have been carried out at a current density of 500 mA.g^{-1} and capacities of 145 mA.h.g^{-1} , 95 mA.h.g^{-1} , and 70 mA.h.g^{-1} have been obtained for $MgMn_2O_4$, $MgNi_2O_4$ and $MgCo_2O_4$, respectively. The theoretical and experimental results show that $MgMn_2O_4$ spinel is the most suitable cathode for magnesium-ion batteries because the magnesium ion diffusion barrier in this structure is lower than other structures. Our research is being done to improve the performance and mechanical stability of these cathodes by using doping solutions of transition elements in the structure and composite with carbon and polymer substrates to achieve commercialization goals.

Biography

Ali Zeinodiny, a Ph.D. student in physical chemistry from Tarbiat Modares University in Iran, who works on energy storage systems such as rechargeable batteries (Li/Multivalent Battery); also have skills in the field of electrochemistry and Python programming



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Accepted Abstracts

SURFACE DEFECT-ENGINEERED CeO_{2-x} BY ULTRASOUND TREATMENT FOR SUPERIOR PHOTOCATALYTIC H_2 PRODUCTION AND WATER TREATMENT

Nabil Alzaqri

King Saud University, Saudi Arabia

Abstract:

Semiconductor photocatalysts with surface defects display incredible light absorption bandwidth and these defects function as highly active sites for oxidation processes by interacting with the surface band structure. Accordingly, engineering the photocatalyst with surface oxygen vacancies will enhance the semiconductor nanostructure's photocatalytic efficiency. Herein, a CeO_{2-x} nanostructure is designed under the influence of low-frequency ultrasonic waves to create surface oxygen vacancies. This approach enhances the photocatalytic efficiency compared to many heterostructures while keeping the intrinsic crystal structure intact. Ultrasonic waves induce the acoustic cavitation effect leading to the dissemination of active elements on the surface, which results in vacancy formation in conjunction with larger surface area and smaller particle size. The structural analysis of CeO_{2-x} revealed higher crystallinity, as well as morphological optimization and the presence of oxygen vacancies is verified through Raman, X-ray photoelectron spectroscopy, temperature-programmed reduction, photoluminescence, and electron spin resonance analyses. Oxygen vacancies accelerate the redox cycle between Ce^{4+} and Ce^{3+} by prolonging photogenerated charge recombination. The ultrasound-treated pristine CeO_2 sample achieved excellent hydrogen production showing a quantum efficiency of 1.125% and efficient organic degradation. Our promising findings demonstrated that ultrasonic treatment causes the formation of surface oxygen vacancies and improves photocatalytic hydrogen evolution and pollution degradation.

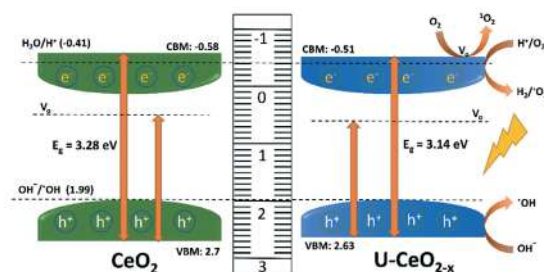


Figure: Energy band positions of CeO_2 and U-CeO_{2-x}

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SYNTHESIS AND CHARACTERISATION OF GO/SrFe₁₂O₁₉ AS MAGNETIC HYBRID NANOCATALYST FOR REGIOSELECTIVE RING-OPENING OF EPOXIDES WITH AMINES UNDER ECO-FRIENDLY CONDITIONS

Laayati Mouhsine, Mekkaoui Ayoub Abdelkader, Bahsis Lahoucine, El Firdoussi Larbi and El Houssame Soufiane

Sultan Moulay Slimane, Morocco

Abstract:

Herein, a highly efficient magnetically separable hybrid GO/SrFe₁₂O₁₉ nanocomposite was synthesized via dispersing M-type strontium hexaferrite (SrFe₁₂O₁₉) on graphene oxide (GO) sheets. First, SrFe₁₂O₁₉ nanoparticles (NPs) and GO sheets were prepared via chemical coprecipitation and chemical oxidation of graphite powder, respectively. Chemically reduced GO (rGO) and rGO/SrFe₁₂O₁₉ were also prepared for a comparison purposes.

Thereafter, the prepared nanostructured materials were explored by XRD, FTIR, Raman, FESEM-EDX, BET, and Zeta-Sizer analyses. All the characterizations confirm the nanoscale and the high stability structures of the prepared materials. The prepared hybrid magnetic nanocomposite GO/ SrFe₁₂O₁₉ exhibited a high surface area value resulting in a high catalytic activity and selectivity for the epoxide ring-opening with amines in neat water. Moreover, the use of hybrid GO/SrFe₁₂O₁₉ compared to the pure SrFe₁₂O₁₉ and GO sheets is of great interest for using environmentally benign heterogeneous nanocatalysts, for the synthesis of β-amino alcohols, with excellent recyclability under eco-friendly conditions. In addition, a mechanistic study was performed through density functional theory (DFT) calculations and Parr functions to explain the observed reactivity and selectivity of SrFe-GO nanocatalyst in epoxide ring-opening reaction.

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March 20-21, 2023 | Rome, Italy



SYNTHESIS, CHARACTERISATION AND INSILICO INVESTIGATION OF CURCUMIN ANALOGUES AS POTENTIAL ANTI CANCER AGENTS

Padminee Ramsaroop

University of the West Indies, Jamaica

Abstract:

Cancer can be defined as a disease in which abnormal cells divide without control and invade nearby tissues. These cells then spread to other parts of the body via the blood and lymph systems. According to The World Health Organization, cancer is the second leading cause of death worldwide and is responsible for an estimated 9.6 million deaths in 2018. While there are many drugs currently on the market, many pose significant adverse side effects. One approach to combat to this issue is the use of Curcumin. Curcumin is a widely used polyphenol in many cultures. It can be extracted from the roots of the plant *Curcuma longa* or can be synthetically made. This plant extract has been shown to exhibit many pharmacological activities including anti-cancer, anti-viral, anti-anxiety, anti-inflammatory, neuroprotective, antioxidant, cardioprotective and anti-fungal properties. While there are many promising aspects of this compound, there are many hurdles that must first be overcome if this compound is to be used as an anti-cancer agent. Among these factors include improving bioavailability, solubility and stability usually faced by free curcumin. This research looks at improving these factors by enhancing the curcumin molecule to create derivatives as well as complexing these derivatives with specific metals to create compounds that can be used as anti-cancer agents. The derivatives would be characterized using techniques such as NMR (^1H , ^{13}C , HSQC, COSY), spectrometry (IR, UV-VIS, Mass, and Fluorescence) and thermogram (melting point and TGA). AMDET profiles will also be looked at for every compound to determine physiological properties and parameters such as medicinal chemistry, absorption, distribution, metabolism, excretion, toxicity, drug likeness and drug score. These compounds will then be tested on various cancer cell lines to determine their effect as well as tested against known agents and free curcumin to determine their efficacy.

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March 20-21, 2023 | Rome, Italy



NEW KINETIC SPECTROPHOTOMETRIC METHODS FOR DETERMINATION OF FLUVASTATIN IN PURE AND PHARMACEUTICAL DOSAGE FORMS

Safwan Ashour

University of Gaziantep, Turkey

Abstract:

New, accurate, sensitive and reliable kinetic spectrophotometric method for the assay of fluvastatin sodium (FVS) in pure form and pharmaceutical formulations has been developed. The method involves the oxidative coupling reaction of FVS with 3-methyl-2-benzothiazolinone hydrazone hydrochloride monohydrate (MBTH) in the presence of Ce(IV) in an acidic medium to form colored product with λ_{max} at 615 nm. The reaction is followed spectrophotometrically by measuring the increase in absorbance at 615 nm as a function of time. The initial rate and fixed time methods were adopted for constructing the calibration curves. The linearity range was found to be 4.0–36.0 $\mu\text{g/mL}$ for initial rate and fixed time methods. The limit of detection for initial rate and fixed time methods is 0.94 and 0.11 $\mu\text{g/mL}$, respectively. Statistical treatment of the experimental results indicates that the methods are precise and accurate. The proposed method has been applied successfully for the estimation of FVS in commercial dosage forms with no interference from the excipients. The obtained results are compared with those of the pharmacopoeial method.

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March 20-21, 2023 | Rome, Italy



FREE RADICALS IN CATALYTIC OXIDATIVE CONVERSION OF METHANE BASED ON IN SITU EPR/MS DATA

Ismailov EH, Taghiyev DB, and Thybaut JW

Institute of Catalysis and Inorganic Chemistry of ANAS, Azerbaijan

Abstract:

Based on EPR spectroscopy data in combination with mass spectroscopy, gas-phase products of oxidative conversion of methane (OCM) were identified and their concentration was studied as a function of temperature and CH_4/O_2 ratio. The data obtained make it possible to consider, within the framework of a unified scheme, all the main stages of this reaction occurring both on the surface and in the gas phase. A stepwise scheme for the oxidation of methane in the presence of oxide catalysts has been proposed. The regularities of the process of reoxidation of OCM catalysts and approaches to the design of spatially separated active particles in multicomponent catalysts responsible for the generation of radical particles and their selective transformation are also considered. Using the $\text{NaMnW}/\text{SiO}_2$ multicomponent oxide catalyst for this reaction as an example, which, according to X-ray phase analysis, consists of MnO_x , Na_2WO_4 , MnWO_4 , and SiO_2 phases, it was shown that at the OCM reaction temperature, i.e., 750-850°C, one of these phases, the Na_2WO_4 phase, is in a molten state (manganese oxides - MnO , Mn_2O_3 , MnO_2 and SiO_2 have a melting point above 850°C), i.e. under the reaction conditions molten Na_2WO_4 with nanosized MnO_x particles and products of their interaction covers the surface of crystalline SiO_2 (with the structure of cristobalite and/or tridymite) in the form of a film. This example demonstrates interesting features of high-temperature reactions, in this case, OCM reactions, catalyzed by multicomponent systems, the components of which are in different aggregate states under the reaction conditions.

This work is funded by the European Union's Horizon 2020 research and innovation program under grant agreement No.814557.

FLUORESCENCE PROPERTIES OF AROMATIC FRAGMENTS CONTAINING PHENANTHRO-IMIDAZOLES

Ayaz Mammadov, Rana Jafarova, Ulviyya Yolchuyeva, Nargiz Orujova and Rufana Mammadova

Azerbaijan National Academy of Sciences, Azerbaijan

Abstract:

Compounds containing heterocyclic and aromatic fragments to have high fluorescent properties have been mentioned in numerous literature sources. Among these compounds, phenanthroimidazoles are especially valued by researchers as fluorophores in the LED industry and in the field of defectoscopy. In the presented work, several phenanthro-imidazoles were synthesized from phenanthrenquinone, ammonium acetate, aromatic amine and aromatic aldehydes using the thermal method in the presence of 1,4 dimethylpiperazinium dihydrosulfate catalyst, and the structures of the compounds were confirmed by IR, ^1H and ^{13}C NMR spectroscopy. The fluorescence properties of the obtained phenanthro-imidazoles were studied in "Cary Eclipse" spectrofluorimeter. Luminescent excitation and photoluminescence spectra were recorded in the wavelength range of 190–1100 nm at room temperature.

4'-(2-phenyl-1H-phenanthro[9,10-d]imidazol-1-yl)-[1,1'-biphenyl]-4-amine. In the absorption spectrum of the sample, the intensity of absorption maxima at 250 and 262 nm related to the π - π^* electron transition is weak and luminescence at the wavelength of 370 nm. Also in the spectrum, the intensity of absorption recorded at wavelengths of 372 and 395 nm, which is related to the n - π^* electron transition, is large. These absorption maxima give luminescence at 406 and 430 nm wavelengths.

4'-(2-(4-(dimethylamino)phenyl)-1H-phenanthro[9,10-d]imidazol-1-yl)-[1,1'-biphenyl]-4-amine. As can be seen from the luminescence spectrum of the substance, the luminescence of excitation at 260 and 262 nm wavelengths was not recorded. Absorption maxima recorded at wavelengths of 354, 372 and 394 nm in the spectrum give luminescence at wavelengths of 406, 430 and 456 nm. Studies have shown that both compounds have coloring properties.

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March 20-21, 2023 | Rome, Italy



SHEEP WOOL KERATIN: A NOVEL DIETARY PROTEIN

George J Dias

University of Otago, New Zealand

Abstract:

Keratin derived protein (KDP) was extracted from sheep wool using high pressure microwave technology developed by the Dias research team, in the presence of food acids (citric and ascorbic), and investigated for its potential as a novel dietary protein. The proximate composition, amino acid profile, mineral profile, in vitro cytotoxicity and digestibility of KDP were evaluated. Nutritive effects of KDP at 50% dietary supplementation was compared with a casein-based control diet in a growing rat model for 95 days. Results indicated KDP to be rich in protein (86%), amino acid cysteine (8.9 g/100 g), arginine (7.4 g/100 g) and glycine (4.2 g/100 g), and minerals selenium (0.29 µg/100 g), and zinc (31.3 µg/100g). KDP was non-cytotoxic in vitro at ≤ 2 mg/mL concentration. There were no differences in the rat weight gain, nor the food consumption compared to the control group ($P > 0.05$). KDP rich food product was scored similar to the control in a sensory trial by the participants. In conclusion, KDP is an effective substitute for casein protein in dietary applications at 50% concentration. Therefore, KDP has the potential to be used in the food industry as a novel dietary protein that is free of fat and carbohydrate. Also, KDP is a cost-effective solution to the challenge of waste wool disposal, and overdependence of other protein sources such as fish meal in livestock feed and aquaculture. Overall, KDP could serve as a relatively cheap and freely accessible solution to the problem of protein malnutrition, especially among low-income groups.

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March 20-21, 2023 | Rome, Italy



TOWARDS THE DEVELOPMENT OF MORE SUSTAINABLE REDOX OF ALCOHOLS AND ALDEHYDES

Mingxin Liu, Chao-Jun Li and Zetian Mi

Lanzhou University, China

Abstract:

Oxidation/reduction are fundamental classes of chemical reactions. Although they play crucial roles in both industry and society, due to the need of stoichiometric oxidant/reductant, the oxidation/reduction often cause extensive energy consumption and waste emission. Devoted to the solution of this problem, our team has discovered the oxidation/reduction of aldehyde/alcohol under air in water, the nitrogen fixation as well as reductive coupling using water/methanol as reductant, and the deoxygenative coupling of methanol into ethanol. The work of us has been highlighted by Science (AAAS), German National Radio, etc. and was commented as "research that could change the world".

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CATALYSIS BY MODIFIED CLAYS: A STATE-OF-THE-ART SURVEY

Pierre Laszlo

University of Liège, Belgium

Abstract:

The talk will focus on recent developments of these superbly-efficient methodologies. As layered aluminosilicates, minerals such as halloysite, hectorite, hydrotalcite, imogolite, laponite, montmorillonite, saponite, vermiculite, etc, clays are turned into catalysts from impregnation or pillaring with various metals, such as iron, cobalt, copper, manganese, titanium, zinc, etc. They bring to this task high specific surface areas, with atomically flat surfaces-a key feature diffusion-wise. Their ability at swelling is another precious aspect. Thus, they can incorporate reactant molecules in their interlamellar spaces.

How did we conceive of catalysis by clays? From their role in prebiotic synthesis of organic molecules, it was logical to assume they might be useful catalysts for present-day chemistry. A feature of the talk will be clay-based green chemistry, such as CO₂ capture, light-harvesting, hydrolysis of pesticides, diesel fuel desulfurization, -and so on.

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Catalysis and Chemical Engineering

March 20-21, 2023 | Rome, Italy



SINGLE ATOM CATALYSTS WITH NANOCONFINED IONIC LIQUIDS FOR ENHANCED CO₂ ELECTROREDUCTION

Qian Sun, Yong Zhao and Chuan Zhao

The University of New South Wales, Australia

Abstract:

Ionic liquids (IL) are effective electrolyte additives that can enhance the electrochemical performances of metallic catalysts for CO₂ reduction reaction (CO₂RR) over. ILs deliver much higher CO₂ solubility than aqueous electrolytes, which can increase the local CO₂ concentration and facilitate CO₂ transportation to the single active site. Besides, ILs can form interaction with CO₂ molecules, lowering the energy barrier for the formation of the key intermediate CO₂. However, ILs typically suffer from high viscosity and expensive costs, leading to slow mass transfer and low conductivity of the electrolytes. Using large quantity of bulk viscous ionic liquids in industrial for CO₂RR electrolyser is impractical.

Here we show a nanoconfined strategy for using ionic liquids for CO₂RR. We confine a hydrophobic ionic liquid (BmimPF₆) into a nickel-nitrogen-carbon (Ni-N-C) single atom catalyst (SAC) to develop a Ni-N-C/ILs nanocomposite catalyst for direct use in aqueous electrolytes for CO₂RR. The synergistic effect between the ILs co-catalyst and Ni-N active sites lead to excellent CO₂RR performances in pure CO₂ and diluted CO₂. The fabricated Ni-N-C/BmimPF₆ exhibited higher CO Faradaic efficiency (FE_{CO}) and partial current densities (j_{CO}) than those of Ni-N-C SAC in pure and diluted (10%, 50%) in a wide potential range from -0.5 to -1.0 V vs RHE. A high FE_{CO} of 98% and a large CO partial current density of 37 mA/cm² were achieved in pure CO₂ on the composite catalyst. This work lay solid foundations for future applications of ionic liquids for industrial CO₂RR and many other important electrochemical reactions such as oxygen reduction reactions, water splitting and nitrogen reduction and beyond.

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March 20-21, 2023 | Rome, Italy



TUNING IMMUNE CELL BIOLOGY WITH MACROCYCLIC GLYCOPEPTIDES

Ryoji Yoshisada, Nadia L van der Meijs, Sandra J van Vliet, and Seino AK Jongkees

Universiteit Amsterdam, Netherlands

Abstract:

Immune responses are shaped through glycan signals. On dendritic cells (DCs), which are a key regulator of the immune system, carbohydrate-specific C-type lectins decode specific sugar patterns of pathogens and glycoproteins. The aim of the project is to find glycopeptides that interact with the receptors to either stimulate or inhibit the functionality. As model cases for this scheme, we take MGL (Macrophage galactose-type lectin) and DC-SIGN (dendritic cell-specific intercellular adhesion molecule-3-grabbing non-integrin), known to recognise GalNAc (N-acetylgalactosamine) and mannose or fucose, respectively. Our approach to finding glycopeptides is by mRNA display incorporating chemical modification of the peptide library with these particular carbohydrates. Here, the role of glycan is not only for binding but for guiding the glycopeptide to the specific binding site. The glycosylation strategy is either 1) click glycosylation between alkyne handle installed at C6 position of the sugar and azidohomoalanine in the peptide or 2) a reaction between a thiol at the C1 position of a sugar and cysteine-derived dehydroalanine in the peptide library. Next to this, we implement peptide macrocyclization either by thioether formation or cyanobenzothiazole reaction with N-terminal cysteine. With such libraries we aim to find new sequences that can bind to C-type lectins and modulate their responses, thereby tuning the biology of dendritic cells.

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March 20-21, 2023 | Rome, Italy



MICRO-KINETICS ANALYSIS BASED ON PARTIAL REACTION NETWORKS TO COMPARE CATALYSTS PERFORMANCES FOR METHANE DRY REFORMING REACTION

Shambhawi, Jana M Weber and Alexei A Lapkin

University of Cambridge, United Kingdom

Abstract:

Designing simple, yet representative reaction network for subsequent micro-kinetic analysis is important for limiting cost of evaluation and ensuring solvability. This is currently achieved by employing sensitivity analysis over a comprehensive reaction network (CRN) to screen reaction species. However, as a reaction network simplifies for a particular catalyst composition, it loses its transferability to other compositions. Therefore, in this study, a two way approach is presented to circumvent this problem. Firstly a generalizable model outcome is identified, i.e. minimum reactant conversions(x_r), based on a mass-flow analysis. Then, a stepwise framework is developed for constructing a partial reaction network (PRN), to insure transferability of $\min(x_r)$ for a range of varying catalyst energetics, in the absence of experimental data for validation. Lastly, the transferability of this approach is demonstrated for CH_4 dry reforming by developing a PRN using Ni(111) as initial catalyst and testing it over Ru(001).

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March 20-21, 2023 | Rome, Italy



ACTIVATION OF PERSULFATES FOR THE REMOVAL OF ENVIRONMENTALLY PERSISTENT POLLUTANTS

Stanisław Waclawek

Technical University of Liberec, Czech Republic

Abstract:

Due to the ubiquitous water pollution, we need to find new water treatment methods that are feasible for specific types of contaminants. Advanced oxidation processes (AOPs) are known for the fast removal of many persistent pollutants from water due to the reactivity of hydroxyl radicals. However, these treatments are still insufficient for removing many complex compounds. A new type of AOPs, SR-AOP are based on sulfate radicals instead of hydroxyl radicals. In SR-AOP, peroxydisulfate (PDS) and peroxymonosulfate (PMS) are common sulfate radical precursors, and their catalytic activation has recently interested environmental engineers and chemists. For example, the mechanism behind forming the reactive oxygen species (ROS) from persulfates is constantly reevaluated. In this presentation, state-of-the-art knowledge will be presented on the persulfates catalytic activation. The influence of pH, water matrix constituents and catalyst type on the ROS formation from persulfates will also be discussed. Further, several reactions between ROS and persistent pollutants in water will be shown. For this, experimental and theoretical investigations will be presented.

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March 20-21, 2023 | Rome, Italy



Note

Forthcoming Events

International Conference on **Biomaterials and Biodevices**

September 25-26, 2023 | Paris, France



2nd International Conference on **Neurology and Brain Disorders**

November 2-3, 2023 | London, UK



Internarional Conference on **Hematology and Blood Disorders**

November 6-7, 2023 | Paris, France



European Conference on **Human Genetics**

November 6-7, 2023 | Paris, France



International Conference on **Gynecology and Obstetrics**

November 6-7, 2023 | Dubai, UAE



International Conference on **Biomedical Science and Engineering**

November 6-8, 2023 | Dubai, UAE



International Confernce on **Clinical Case Reports**

November 8-9, 2023 | Dubai, UAE



2nd International Conference on **Materials Science & Engineering**

November 8-9, 2023 | Dubai, UAE



2nd European Congress on **Chemistry and Applied Sciences**

November 9-10, 2023 | Paris, France



2nd International Conference on **Catalysis & Chemical Engineering**

November 9-10, 2023 | Paris, France



European Congress on **Renewable Energy and Sustainable Development**

November 16-17, 2023 | Rome, Italy



European Congress on **Biopolymers and Bioplastics**

November 16-17, 2023 | Rome, Italy



2nd International Conference on **Nanomaterials and Nanotechnology**

November 20-21, 2023 | Vienna, Austria



2nd European Congress on **Microbiology**

November 20-21, 2023 | Vienna, Austria



2nd International Conference on **Infectious Diseases**

November 20-21, 2023 | Vienna, Austria



2nd International Conference on **Addiction & Psychiatry**

November 20-21, 2023 | Vienna, Austria

