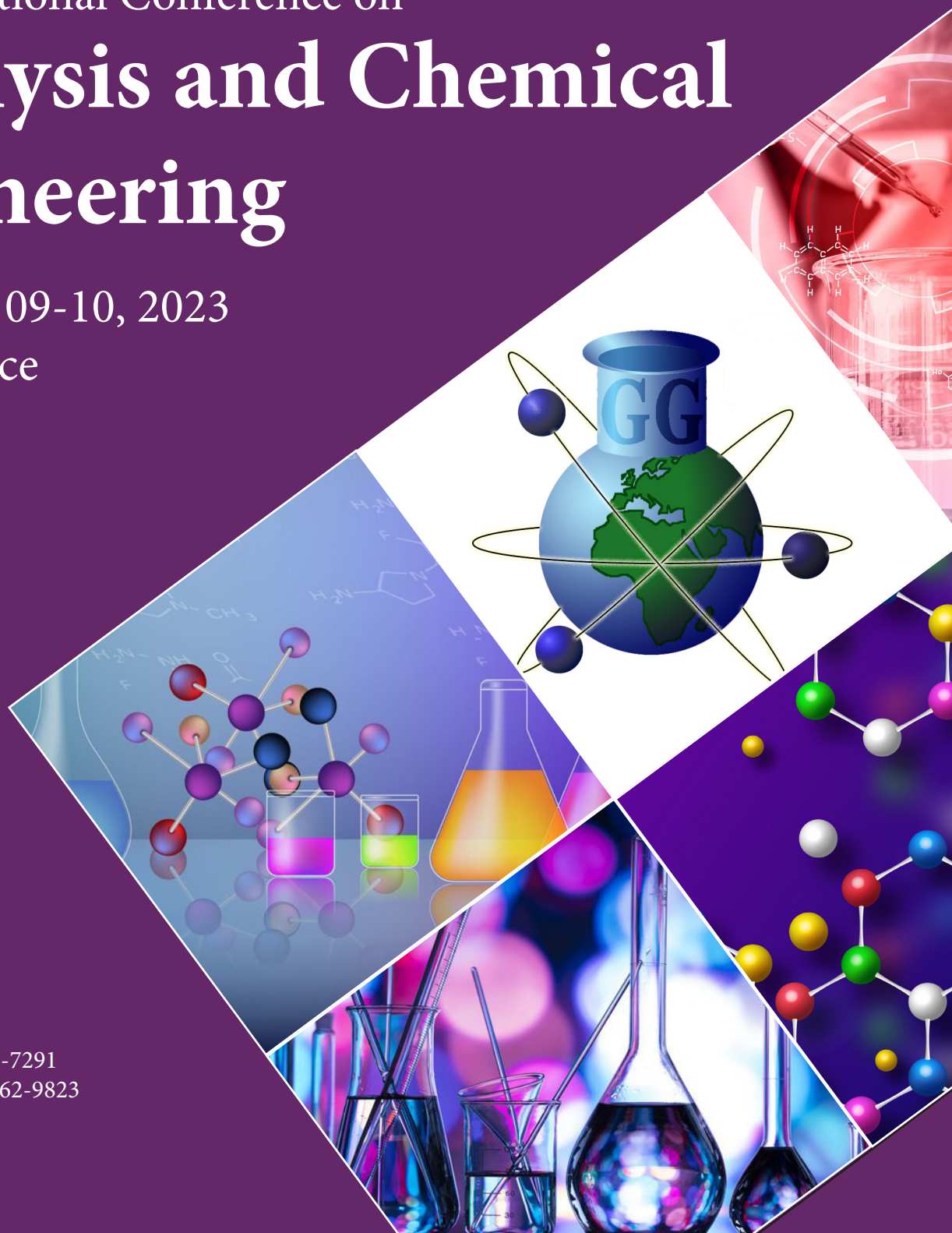


# Chemistry and Applied Sciences

# Sciences & 2<sup>nd</sup> International Conference on Catalysis and Chemical Engineering

November 09-10, 2023

# Paris, France



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# Conference Programme

# Conference Programme

November 09-10, 2023, Millennium Hotel Paris Charles De Gaulle, Paris, France

## Day 1, November 09, 2023

### Meeting Hall: Bleriot

8.00 - 8.45

Registrations

8.45 - 9.00

Introduction

### Keynote Presentations

9.00 - 9.40

Stanislaw Dzwigaj, Sorbonne Université, France

Title: CO<sub>2</sub>-Assisted Dehydrogenation of Propane to Propene over Zn-BEA Zeolites: Impact of Acid-Base Characteristics on Catalytic Performance

9.40 - 10.20

Renato Tomaš, University of Split, Croatia

Title: Ionic liquids: My Research Contribution

### Group Photo: 10.20 - 10.40

### Networking and Refreshments : 10.40 - 11.00 @ Foyer

11.00 - 11.40

Mirta Rubcic, University of Zagreb, Croatia

Title: Dihydrazones and Carbohydrazides: A Fruitful Platform for the Development of Multifunctional Materials

### Oral Presentations

Session Chair:

Stanislaw Dzwigaj, Sorbonne Université, France

Session Chair:

Višnja Vrdoljak, University of Zagreb, Croatia

**Sessions:** Catalysis for Chemical Synthesis | Chemical Engineering | Catalysis for Energy | Materials Chemistry and Catalysis | Catalysis and Zeolites | Catalysis and Pyrolysis | Physical Chemistry | Organic Chemistry | Photocatalysis and Electrochemistry | Catalysis for Renewable Sources | Green & Sustainable Chemistry | Advanced Synthesis and Catalytic Systems | Polymer Science and Technology | Enzymes and Biocatalysts | Catalysis in Oil & Gas and Petrochemical Engineering | Fluid Dynamics & its Phenomena | Environmental Catalysis | Simulation and modelling in Catalysis

11.40 - 12.05

Felix Panis, University of Vienna, Austria

Title: Tyrosinases: Ticking Time Bombs in Wetland Ecosystems!

12.05 - 12.30

**Višnja Vrdoljak**, University of Zagreb, Croatia

Title: Hybrid Organic-Inorganic Compounds based on the Polyoxomolybdate and Dioxomolybdenum(VI) Complexes: Synthesis, Structure, and Properties

12.30 - 12.55

**Vahide Nuran MUTLU**, SOCAR Turkey Research & Development and Innovation, Turkey

Title: Electrocatalytic Hydrogenation of Acetone to Isopropanol over Mesoporous Carbon Supported Bimetallic Catalysts for LOHC Applications

**Lunch @ Restaurant: 12.55 - 14.00**

14.00 - 14.25

**Nedyalka Valcheva**, Trakia University, Bulgaria

Title: Physical, Chemical, and Microbiological Characteristics of Mineral, Mountain, and Spring waters from Bulgaria, and Biological Properties of Identified Microorganisms

14.25 - 14.50

**Sneha Sandeep Lavate**, Pandit Deendayal Energy University, India

Title: One Pot Synthesis of 2D/0D VCu Layered Double Hydroxide/TiO<sub>2</sub> Nanoparticles for Electrochemical CO<sub>2</sub> Reduction to Hydrocarbons

14.50 - 15.15

**Ruaraidh Wells**, NiTech Solutions Ltd, United Kingdom

Title: Continuous Production of a Functional Consumer Care Product through Process Innovation

15.15 - 15.40

**Jacek Siódmiak**, Bydgoszcz University of Science and Technology, Poland

Title: An Investigation of Seed Mucilage Network Properties and its Formation Process using Computer Modelling

15.40 - 16.05

**Radha N Somaiya**, IIT-BOMBAY, India

Title: Promising Quasi-2D PdSi<sub>2-x</sub>Ge<sub>x</sub>N<sub>4</sub> (x = 0, 1, 2) candidate for Spontaneous Overall Water Splitting

**Networking and Refreshments: 16.05- 16.30 @ Foyer**

16.30 - 16.55

**Aysel Zahidova**, SOCAR Turkey Research & Development and Innovation, Turkey

Title: Turning CO<sub>2</sub> from a Liability into an asset with the help of Catalysis

16.55 - 17.20

**Iman Ahmed Youssef Ghannam**, National Research Centre-  
Dokki, Egypt

Title: Discovery of PPAR Agonists as Therapeutics in Metabolic Disorders

17.20 - 17.45

**Wafaa Lounis**, University Oran 1 ABB, Algeria

Title: Flaxseed Oil effect in Improving Neurological Impairments in Rat Pups intoxicated by Aluminum

## Day 1 Concludes followed by Awards Ceremony

**Day 2, November 10, 2023**

**Meeting Hall: Bleriot**

## Keynote Presentations

9.00 - 9.40

**Omar Chaalal**, Abu Dhabi, UAE

Title: Global Green Integrated Process

9.40 - 10.20

**Irena Kostova**, Medical University-Sofia, Bulgaria

Title: Synthesis, Theoretical and Spectral Characterization of Biologically Active Lanthanide(III) Complexes

10.20-11.00

**Rohit Srivastava**, Pandit Deendayal Energy University, India

Title: Exploring Enhanced Two-Dimensional Advance Electrocatalyst for the Production of Green Hydrogen: Approaches to Achieving Corrosion Resistance in Seawater Electrolysis

## Networking and Refreshments: 11.00 - 11.30 @ Foyer

## Oral Presentations

Session Chair:

**Irena Kostova**, Medical University-Sofia, Bulgaria

Session Chair:

**Omar Chaalal**, Abu Dhabi, UAE

**Sessions:** Chromatography & Mass Spectrometry | Nuclear and Radio Chemistry | Drug Chemistry | Biochemistry | Pharmaceutical Chemistry | Organic chemistry | Geochemistry | Food chemistry | Inorganic Chemistry | Food science | Agricultural Sciences | Renewable Energy | Medicinal Chemistry | Physical Chemistry | Analytical Chemistry | Nanomaterials | Chemical Engineering | Polymer Chemistry | Natural Products and Peptide Chemistry | Applied Chemistry

11.30-11.55

**Juhi Saraswat**, Jamia Millia Islamia, India

Title: Synergistic effect of N-substituted Pyrrolidinium based-ionic liquids on AMP:Strategy to Combat Bacterial Resistance

11.55-12.20

**Zahra Akbari**, University of Messina, Italy

Title: Determination of Lead ions ( $\text{Pb}^{2+}$ ) on Schiff base Ligand L-based SPCE electrode in Seawater

12.20-12.45

**Grigorii Buklei**, HSE University, Russia

Title: Efficient Data Acquisition Optimization for Chemical Kintetics: Leveraging Orthogonal Decision Trees and Machine Learning

12.45 - 13.10

**Aashima Anand**, Jamai Millia Islamia, India

Title: Optimization and Characterization of Ionic Liquid – Surfactant based Nanoemulsions for Effective Pesticide Utilization

### **Lunch @ Restaurant: 13.10 - 14.00**

14.00-14.25

**Mamadou Simina Drame**, Université Cheikh Anta Diop de Dakar, Sénégal

Title: Assessment of Natural and Anthropogenic Contributions Particulate Matter Air Pollution in Dakar, Senegal

14.25-14.50

**Lozan Todorov**, Medical University – Sofia, Bulgaria

Title: Antioxidant Properties of a Novel Triazole Ligand and its Lanthanide(III) Complexes

14.50-15.15

**Aleksandra Jankowska**, Jagiellonian University, Poland

Title: Copper-Modified Heteroatomic Ce-MWW Zeolites as Potential NO Conversion Catalysts

### **Poster Presentations**

Poster -01

**Noura Benlemlih**, University of Ibn Tofail , Morocco

Title: The Potential for Utilizing Sludge from the Kenitra Wastewater Treatment Plant in Agricultural Practices

Poster -02

**Aleksandra Gomulka**, Jagiellonian University, Poland

Title: Effective Catalysts for Low-Temperature  $\text{NH}_3$ -SCR Process based on Copper-Modified MCM-41 Mesoporous Silica - Comparison of TIE and ADP Methods



**Poster -03**

**Wafaa Lounis, University Oran 1 ABB, Algeria**

Title: Flaxseed Oil effect in Improving Neurological Impairments in Rat Pups intoxicated by Aluminum

**Poster -04**

**Safae EL AAMMOURI, University of Ibn Tofail , Morocco**

Title: Wastewater Treatment by Infiltration Percolation Process using Fine Sand and Activated Carbon

**Poster -05**

**Wiktorja Dubiel, Jagiellonian University, Poland**

Title: The Effect of Iron addition in Silica-Titania Mesoporous Catalysts on the Efficiency of the Diphenyl Sulfide Oxidation Process

**Poster -06**

**Zehor Chouari, University Oran ABB, Algeria**

Title: Prophylactic Role of Cafeic Acid against Aluminum-Induced Kidney Damage in Wistar Rats

**Poster -07**

**Vivian García Rojas, Universidad de La Serena, Chile**

Title: Evaluation of Blueberry Pomace for the Production of Antioxidant Compounds through Enriched Natural Fermentation

**Networking and Refreshments : 16.00 - 16.30 @ Foyer**

**Video presentations**

**VP001**

**Diego Tomassone, Holos Medical Clinical and Research, Italy**

Title: The Vitamin D, IL-6 and the eGFR Markers a Possible Way to Elucidate the Lung-Heart-Kidney Cross-Talk in COVID-19 Disease: A Foregone Conclusion

**VP002**

**Vivian García Rojas, Universidad de La Serena, Chile**

Title: Fermentation with Native Microorganisms in Raw, Bleached and Sterilized Broccoli Puree as a Strategy to increase the Sulforaphane Content

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



# Virtual Programme

**Day 1 November 09, 2023 GMT (London Time: 11.00 - 17.00)**

## Oral presentations

11.00-11.25

**Joanna Drzeżdżon**, University of Gdansk, Poland

Title: The Catalytic Role of Acetylacetonate Complex Compounds of Vanadium(IV) in the Polymerization of Selected Olefins

11.25-11.50

**Santoshi Misra**, St. Ann's College for Women- Hyderabad, India

Title: Enhancement of Thermal Conductivity and Heat Transfer rate involving Hybrid Nano Fluids on MHD Stagnation Point Flow over a Stretching Sheet

11.50-12.15

**Tjandra Chrismadha**, National Research and Innovation Agency, Indonesia

Title: Development of Outdoor Inclined Photobioreactor for *Arthrospira Platensis* Culture: Controlling Solar Irradiance to Enhance the Productivity

12.15-12.40

**Menouar HANAFI**, The University of Science and Technology of ORAN, Algeria

Title: The Study of the Catalytic Reforming Plant and the Production of the Gasoline in the Petroleum Refinery of Arzew-Algeria

12.40-13.05

**Evgeny Kabachkov**, Russian Academy of Sciences, Russian Federation

Title: Enhanced Catalytic Activity of Pt/Tin Nanocomposites for CO Oxidation at Low Temperatures

**Lunch(13.05-14.00)**

## Keynote presentations

14.00 - 14.40

**Anne M. Gaffney**, University of South Carolina, USA

Title: Plastic Trash to Monomers and Intermediates – PTMI

14.40 - 15.20

**Haibo Ge**, Texas Tech University, USA

Title: Directed C-H Functionalization of Common Organic Framework

## Oral presentations

15.20-15.45

**Ashanendu Mandal**, University of Calcutta, India

Title: Wastewater Treatment for Removal of Toxic Phenol using Biological and Industrial Wastes as Adsorbents

15.45-16.10

**Muhammad Zubair**, Quaid-I-Azam University, Pakistan

Title: Catalyst for Biofuel Production

16.10-16.35

**Mohammed Hadi Dehgani**, Tehran University of Medical Sciences, Iran

Title: 4-Chlorophenol Adsorption from Water by Activated Carbon Functionalized with Amine Groups

16.35-17.00

**Amir Sepehri**, Islamic Azad University, Iran

Title: Ceiling Graphene: Wireless system

**Day 1 Concludes followed by Awards Ceremony**

**Day 2 November 10, 2023 GMT (London Time: 11.00 - 14.10)**

### **Keynote presentations**

**11.00 - 11.40**

**Osman Adiguzel, Firat University, Turkey**

Title: Shape Reversibility and Crystallographic Transformations in Shape Memory Alloys

### **Oral presentations**

**11.40-12.05**

**Salih Indad, Salahaddin University, Iraq**

Title: Change of the Fractional Composition of Resins and Asphaltenes from High Viscosity Oil in the Process of Catalytic Aquathermolysis

**12.05-12.30**

**Moustapha Kébé, University Cheikh Anta Diop Dakar, Senegal**

Title: Analysis of Black Carbon Concentrations in  $PM_{2.5-10}$  and  $PM_{2.5}$  Fractions by MABI Instrument in Two Urban Areas of Dakar, Senegal

**12.30-12.55**

**Wilbert Mtangi, Chinhoyi University of Technology, Zimbabwe**

Title: Chiral Photoelectrodes for Efficient Water Splitting

**12.55-13.20**

**Firouz Matloubi Moghaddam, Sharif University of Technology, Iran**

Title: Synthesis and Catalytic Application of Magnetic Metal Ferrite Nanoparticles in Organic Reactions

**13.20-13.45**

**Djedouani Djamila, USTHB, Algeria**

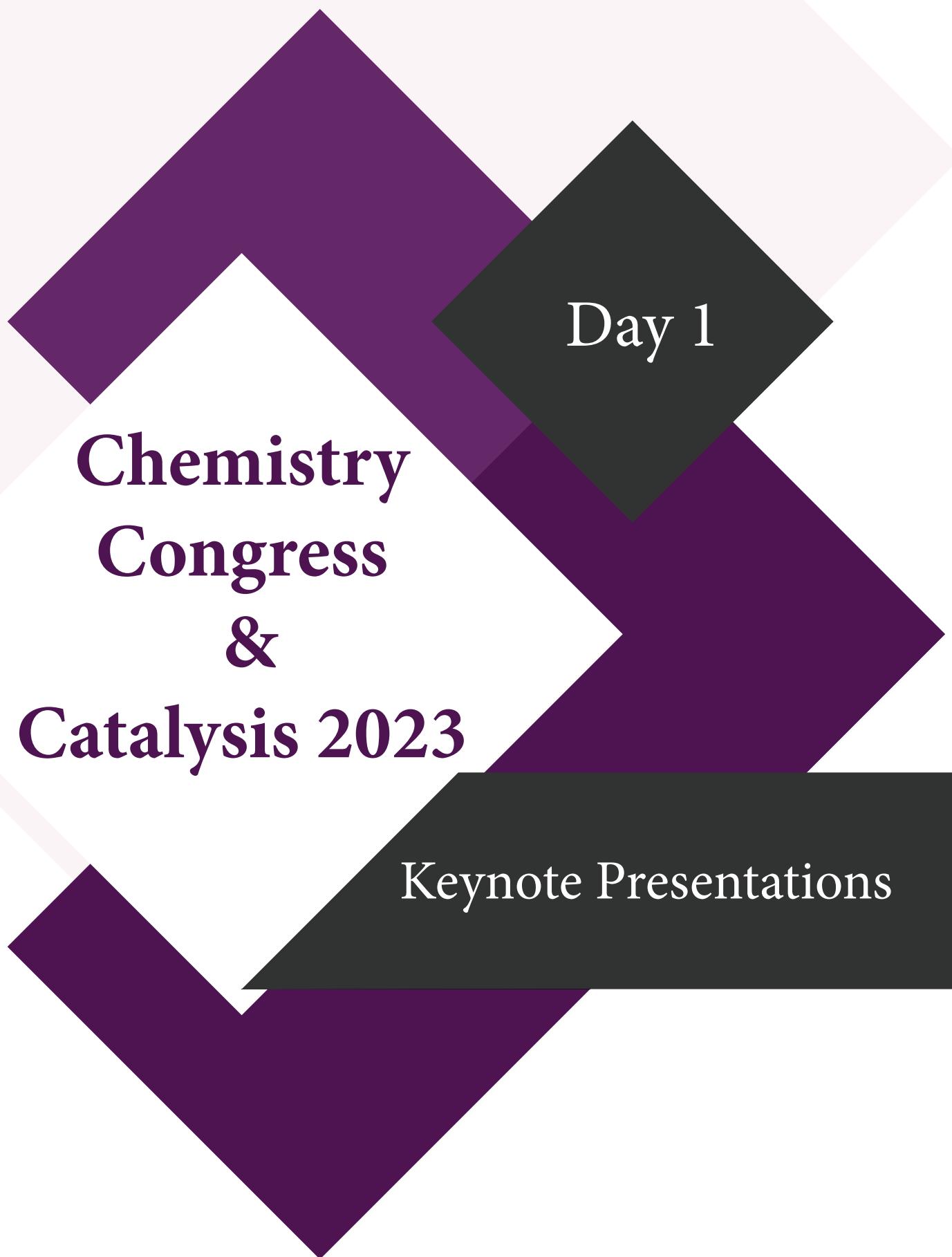
Title: Mass Transfer Coefficients Evaluation of Oxytetracycline Catalysis: Diffusion through  $TiO_2$ /Synthesized Activated Carbon Composites Problem State

**13.45-14.10**

**Suresh Aluvihara, University of Peradeniya, Sri Lanka**

Title: An Advanced Review on the Contaminations of Water in Leather and Footwear Manufacturing Industry and Appropriate Treatment Methods





Day 1

**Chemistry  
Congress  
&  
Catalysis 2023**

Keynote Presentations

2<sup>nd</sup> European Congress on

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# Catalysis and Chemical Engineering

November 09-10, 2023 | Paris, France



## CO<sub>2</sub>-ASSISTED DEHYDROGENATION OF PROPANE TO PROPENE OVER Zn-BEA ZEOLITES: IMPACT OF ACID-BASE CHARACTERISTICS ON CATALYTIC PERFORMANCE



**Stanislaw Dzwigaj**

*Sorbonne Université, France*

### Abstract:

Research results about the influence of BEA zeolite preliminary dealumination on the acid–base characteristics and catalytic performance of 1% Zn-BEA compositions in propane dehydrogenation with CO<sub>2</sub> are presented. The catalyst samples, prepared through a two-step post-synthesis procedure involving partial or complete dealumination of the BEA specimen followed by the introduction of Zn<sup>2+</sup> cations into the T-positions of the zeolite framework, were characterized using XRD, XPS, MAS NMR, SEM/EDS, low-temperature N<sub>2</sub> ad/desorption, C<sub>3</sub>H<sub>8</sub>/C<sub>3</sub>H<sub>6</sub> (CO<sub>2</sub>, NH<sub>3</sub>)-TPD, TPO-O<sub>2</sub>, and FTIR-Py techniques. Full dealumination resulted in the development of a mesoporous structure and specific surface area (BET) with a twofold decrease in the total acidity and basicity of Zn-BEA, and the formation of Lewis acid sites and basic sites of predominantly medium strength, as well as the removal of Brønsted acid sites from the surface. In the presence of the ZnSiBEA catalyst, which had the lowest total acidity and basicity, the obtained selectivity of 86–94% and yield of 30–33% for propene (at 923 K) exceeded the values for ZnAlSiBEA and ZnAlBEA. The results of propane dehydrogenation with/without carbon dioxide showed the advantages of producing the target olefin in the presence of CO<sub>2</sub> using Zn-BEA catalysts.

### 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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# Catalysis and Chemical Engineering

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## IONIC LIQUIDS: MY RESEARCH CONTRIBUTION



**Renato Tomaš**

*University of Split, Croatia*

### Abstract:

Ionic liquids (ILs), as material of the future, in principle are a diverse group of salts which are mostly liquid at ambient temperature. The properties of ILs such as low vapour pressure, high thermal stability, electroactivity, high electrical conductivity, non-flammability and extensive liquid range, anti-microbial properties, unusual solvation properties, highly tunable properties by cation and anion variation and combination promote them as “green” solvents. Therefore, ILs are not only interesting for the scientific community, but have industrial application as well (e.g. IL + organic solvent mixtures as potential optimal electrolytes for lithium-ion batteries). Over the two past decades, ILs have become one of the fastest growing media for chemists and engineers due to their superb physicochemical properties. These liquids can be used as heat transfer fluids, lubricants, electrolytes, liquid crystals, for mercury and CO<sub>2</sub> capture, solar thermal conversion, or in biofuel production. In this presentation I will report my recent results for thermodynamic and transport properties of ILs in various solvents at different temperatures. This lecture will also discuss about some methods of investigation such as conductometry, volumetry and viscometry for solution chemistry study.

### Biography

Renato Tomaš was born 1967 in Trogir, Croatia. He graduated in chemical technology at the Faculty of Chemistry and Technology, University of Split, Croatia. In October, 2002 he obtained the title of PhD at the same University. He holds course of Physical Chemistry for students of chemistry, food technology and pharmacy. He is also lecturer for Selected Topics in Physical Chemistry of Environmental to PhD students of chemistry. His scientific work is connected with solution chemistry (thermodynamic and transport properties of electrolytes), calixarene chemistry, and investigation of ionic liquids. He published about 40 scientific papers and participated in numerous international conferences. He was active in numerous research projects, and currently he is involved in the COST project, EU: Network for Equilibria and Chemical Thermodynamics Advanced Research (NECTAR). He is a member of Croatian Chemical Society.



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## DIHYDRAZONES AND CARBOHYDRAZIDES: A FRUITFUL PLATFORM FOR THE DEVELOPMENT OF MULTIFUNCTIONAL MATERIALS



**Mirta Rubčić, Edi Topić, Jana Pisk, and Višnja Vrdoljak**

*University of Zagreb, Croatia*

### Abstract:

The hydrazone  $R_1R_2C=N-NHR_3$  functionality is a widespread building block, incorporated in a multitude of organic and metal-organic systems. Its structural modularity, stability and adaptability towards the environment allows hydrazones to act as sensors, molecular switches, and/or as anion receptors. On the other hand, the prospect of their *E/Z* isomerization makes them adequate for the development of metal-organic assemblies with stimuli-responsive features.

Within this family of compounds highly intriguing are those derived from carbohydrazides and dihydrazides. Namely, based on the synthetic path the obtained products can be unsymmetrical or symmetrical, thus providing a fruitful platform for the development of functional organic or metal-organic materials.

In this talk synthetic opportunities towards symmetrical and unsymmetrical carbohydrazides/dihydrazones as well as towards their metal-organic assemblies will be discussed. Furthermore, relevant examples of the organic and metal-organic materials of this class will be given and reasoned in terms of their solid-state and solution behavior.

### Biography

Mirta Rubčić obtained her PhD in 2008 at the Faculty of Science, University of Zagreb, and spent a year as a post-doc at Bielefeld University, Germany, at prof. dr. dr. h. c. mult. A. Müller's lab. She is currently working as a Full Professor at the Department of Chemistry, Faculty of Science, University of Zagreb. Her research interests include solid-state chemistry of organic, inorganic and hybrid organic-inorganic compounds. She has expertise in thermal analyses, X-ray diffraction as well as IR, Raman and NMR spectroscopy. She is highly interested in contemporary topics of crystal engineering of functional materials and chemical crystallography.



Day 1

**Chemistry  
Congress  
&  
Catalysis 2023**

Oral Presentations

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November 09-10, 2023 | Paris, France



## TYROSINASES: TICKING TIME BOMBS IN WETLAND ECOSYSTEMS!

**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. Wetlands store of  $550 \times 10^{15}$  g of carbon, which is equivalent to 73% of the atmospheric carbon pool. Phenolic compounds represent recalcitrant molecules naturally present in wetlands which are crucial for the preservation of wetland carbon stores as they act as broad-scale inhibitors of hydrolytic enzymes. Tyrosinases are among the few enzymes capable of removing phenolic compounds in the presence of  $O_2$ . In the wake of climate change an increased aeration of previously anoxic wetland soils has become a likely scenario, which will boost tyrosinase activity, remove phenolic compounds and, thus, threaten the stability of wetland carbon stores. Within recent decades, the biochemical properties of 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. This pioneering research straddles these two previously separated research areas. First, a phylogenetically diverse set of tyrosinase-producing bacteria indigenous to globally distributed wetland ecosystems and their corresponding tyrosinase enzymes has been identified. Second, using five recombinantly expressed wetland-tyrosinases, it has been demonstrated that tyrosinase 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). Third, the impact of increased tyrosinase activity on wetland soils has been investigated for the first time using recombinantly expressed wetland-tyrosinases. This revealed two competing mechanisms describing how increased tyrosinase activity will threaten the stability of wetland carbon stores. Taken together, these results underline the important role of tyrosinases as key enzymes controlling carbon storage in wetland ecosystems.

### Biography

Felix Panis successfully completing his master's studies in pharmacy in 2015, Felix Panis has started his PhD 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 PhD studies and is currently being progressed during his postdoctoral research employment. In 2023, Felix Panis has been granted an ESPRIT-fellowship by the Austrian Science Fund for his excellent environmental research. 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.

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## HYBRID ORGANIC–INORGANIC COMPOUNDS BASED ON THE POLY-OXOMOLYBDATE AND DIOXOMOLYBDENUM(VI) COMPLEXES: SYNTHESIS, STRUCTURE, AND PROPERTIES

**Višnja Vrdoljak, Mirna Mandarić, Nikol Bebić, Jana Pisk, Edi Topić, Mirta Rubčić, Marina Cindrić and Tomica Hrenar**

*University of Zagreb, Croatia*

### Abstract:

Polyoxometalates (POMs) have attracted attention in many fields of science due to their structural versatility, compositional adjustability, and chemical features. Studies have been focused on their structural modifications through transition metal complexes or organic component introduction. Such hybrid compounds exhibit unique properties depending on the counter-ions, metal oxo-cluster constituents, oxidation state of metals, and ligand features. In part, our work has been directed toward research of such Mo<sup>VI</sup> organic–inorganic POM-based hybrids.

We selected hydrazones as organic ligands as they have a propensity for reversible protonation and deprotonation and represent a good starting point for a hybrid generation. The assembly of Mo<sup>VI</sup>O<sub>2</sub><sup>2+</sup> units and organic components allowed the formation of two hybrid classes. In *Class I* assemblies, having the general composition [MoO<sub>2</sub>(HL)(D)]<sub>2</sub>[Mo<sub>6</sub>O<sub>19</sub>] or [MoO<sub>2</sub>(HL)(D)]<sub>4</sub>[Mo<sub>8</sub>O<sub>26</sub>] (D = CH<sub>3</sub>COCH<sub>3</sub>, H<sub>2</sub>O, or CH<sub>3</sub>CN), hydrazonato ligands or their Mo<sup>VI</sup>-complex cations define the network into which the POM anions are embedded, and electroneutrality is achieved. In this way, the cations appear to trigger the hybrid formation through different interactions, electrostatic, van der Waals, or hydrogen bonds. The *Class II* hybrids contain POM anion covalently anchored to two peripheral Mo-complex units through the Mo–O<sup>t</sup>=Mo<sub>POM</sub> linkages, as found in [{MoO<sub>2</sub>(HL)}<sub>2</sub>Mo<sub>6</sub>O<sub>19</sub>] or [{MoO<sub>2</sub>(H<sub>2</sub>L)}{MoO<sub>2</sub>(HL)}Mo<sub>8</sub>O<sub>26</sub>{MoO<sub>2</sub>(HL)}]. Their formation relies almost entirely on the structure-directing effects of the metal-organic components and chosen solvents.

*Class I* and *II* hybrids were generally prepared using conventional and solvothermal synthesis, respectively. A neat and liquid-assisted ball-mill grinding approach was undertaken as an alternative route for *Class II* hybrids. All POM-hybrids were fully characterized. Finally, we used quantum chemical calculations to evaluate the impact of the metal-organic components on the particular hybrid-type formation. *Class II* architectures were also tested as catalysts for cyclooctene epoxidation. Compounds with longer Mo–O<sup>t</sup> bond distances were the best performing hybrids in the *Class II* series.

### Biography

Višnja Vrdoljak received her Ph.D. 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, metallasupramolecular 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.

## ELECTROCATALYTIC HYDROGENATION OF ACETONE TO ISOPROPANOL OVER MESOPOROUS CARBON SUPPORTED BIMETALLIC CATALYSTS FOR LOHC APPLICATIONS

Vahide Nuran MUTLU<sup>1</sup>, Yağmur ÇETİN<sup>2</sup> and Başar ÇAĞLAR<sup>2</sup>

<sup>1</sup>SOCAR Turkey Research & Development and Innovation Inc Aliaga, Turkey

<sup>2</sup>Izmir Institute of Technology, Department of Energy Systems Engineering, Turkey

### Abstract:

Isopropanol's versatile properties and extensive industrial applications underscore its significance in various sectors. Its role as a solvent, fuel additive, antifreeze agent, and pharmaceutical intermediate has led to a robust market demand. Consequently, finding sustainable methods for isopropanol synthesis holds substantial importance. Commercial production of isopropanol is performed by indirect hydration of refinery-grade propylene or direct hydration of chemical-grade propylene. Both of these processes have their own drawbacks such as corrosion problems, waste management, environmental issues and high operation costs due to the high temperature and pressure requirements. The electrochemical hydrogenation (ECH) of acetone to isopropanol offers a promising alternative to traditional thermochemical approaches. Despite its potential, this electrochemical route faces challenges such as selectivity, catalyst stability, and energy efficiency. On the other hand, as hydrogen emerges as a clean and efficient energy carrier, hydrogen storage becomes a critical challenge. Liquid Organic Hydrogen Carriers (LOHCs) have emerged as a viable solution, enabling safe and efficient hydrogen storage and release. Isopropanol, with its high hydrogen content, becomes an attractive candidate for LOHC applications. The reversible hydrogenation and dehydrogenation of isopropanol can facilitate the on-demand release of hydrogen for various applications, including fuel cells and power generation. Isopropanol might also be used in Direct Isopropanol Fuel Cells (DIFCs) which offer a direct electrochemical pathway for harnessing the energy stored in isopropanol without the need for external reforming processes. This direct conversion offers potential advantages in terms of efficiency and simplicity compared to traditional hydrogen fuel cells. Challenges such as catalyst development, reaction kinetics, and system optimization, however, need to be addressed for the widespread adoption of DIFCs. This study focused on the cathode side and studied electrocatalytic hydrogenation (ECH) of acetone in the presence of mesoporous carbon supported Cu-based bimetallic catalysts. The effect of second metal (Co, Ni, Pt) and its composition on the activity, selectivity and stability in a divided cell was investigated via cyclic voltammetry, electrochemical impedance spectrometry (EIS) and chronoamperometry. The results will be presented and discussed and the potential of acetone-water electrolyzer will be evaluated as an energy storage alternative.

### Biography

Vahide MUTLU is a Process Development Supervisor in SOCAR Türkiye Research & Development and Innovation. She got her PhD in Chemical Engineering, M.Sc in Material Science and Engineering, and B. Sc in Chemical Engineering at Izmir Institute of Technology, Türkiye where, she worked as a research assistant for 9 years. Her research interests are design & synthesis of solid catalysts, catalytic conversion of biomass to chemicals, catalytic processes and materials for renewable energy and chemical synthesis. She has expertise in catalyst preparation and characterization and reaction engineering.



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# Catalysis and Chemical Engineering

November 09-10, 2023 | Paris, France



## PHYSICAL, CHEMICAL, AND MICROBIOLOGICAL CHARACTERISTICS OF MINERAL, MOUNTAIN, AND SPRING WATERS FROM BULGARIA, AND BIOLOGICAL PROPERTIES OF IDENTIFIED MICROORGANISMS

**Nedyalka Valcheva**

*Trakia University, Bulgaria*

### Abstract:

There are many mineral, healing, and spring waters in Bulgaria, which are not subject to physicochemical and microbiological control but are used for the drinking needs of the population. Similar water sources are located in almost all regions in the country. Microorganisms with valuable properties and biologically active substances have been found in many minerals, hyperthermal, thermal, and non-thermal spring waters worldwide and in our country. This opens up a new opportunity for researchers to isolate and identify new microorganisms that may apply to people's lives. The aim of the investigation was to study the physical, chemical, and microbiological characterization of mineral, mountain, and spring waters from Bulgaria and the biochemical analysis of the microorganisms identified. Physical, chemical, and microbiological characterization of 90 mineral, mountain, and spring waters from 11 regions in the country – Haskovo, Stara Zagora, Yambol, Sliven, Burgas, Varna, Plovdiv, Pazardzhik, Sofia, Lovech, and Blagoevgrad – was carried out. Molecular genetic identification of 91 isolated microorganisms from 90 mineral, mountain, and spring waters from 11 regions of the country was carried out for the first time. They belong to the following eight genera: *Bacillus*, *Brevibacillus*, *Geobacillus*, *Aeromonas*, *Klebsiella*, *Pseudomonas*, *Staphylococcus*, and *Stenotrophomonas*. The enzyme (amylolytic, proteolytic and lipolytic) and antimicrobial activities against saprophytic and pathogenic microorganisms of the identified microorganisms were determined. The adhesive ability to human epithelial cells was determined for the first time. With the most significant anti-inflammatory, immunomodulatory properties, i.e., with the most substantial inhibition of the production of the cytokine IL-8 (pg/mL) and induction of the synthesis of transforming growth factor beta TGF-beta (pg/mL) are strains *Bacillus subtilis* 0-2 and *B. thuringiensis* B62. These two strains are potentially promising as probiotics alone or in combination with lactic acid bacteria to enhance probiotic activity, anti-inflammatory properties, and to be used in biotechnological production.

### Biography

Nedyalka Valcheva from 1990, she completed his Master's degree program of "Technology of vegetable, food and flavor products" in University of Food Technologies, town Plovdiv, Bulgaria. From 1990 to 2016, she worked as a lecturer at the Vocational High School of Chemical and Food Technologies "Prof. Asen Zlatarov, PhD., town Dimitrovgrad, Bulgaria. From 2014 - the dissertation on "Microflora of healing and spring waters in the Haskovo and Stara Zagora regions" at University of Food Technologies, town Plovdiv with a Ph.D degree. Since 2016, she working as a senior expert, organizer in Department of Biochemistry, Microbiology and Physics in Trakia University, town Stara Zagora, Bulgaria. From 2023 - the dissertation on " Physical, chemical, and microbiological characteristics of mineral, mountain, and spring waters from Bulgaria, and biological properties of identified microorganisms" at Institute of Cryobiology and Food Technologies, Agricultural Academy, town Sofia, Bulgaria with a DSc.

## ONE POT SYNTHESIS OF 2D/0D VCU LAYERED DOUBLE HYDROXIDE/TIO<sub>2</sub> NANOPARTICLES FOR ELECTROCHEMICAL CO<sub>2</sub> REDUCTION TO HYDROCARBONS

**Sneha Sandeep Lavate, and Rohit Srivastava**

*Pandit Deendayal Energy University, India*

### Abstract:

Although typically considered a combustion byproduct, carbon dioxide (CO<sub>2</sub>) could potentially serve as a valuable feedstock for the production of both fine and commercially viable organic compounds, given the availability of an effective method. The concept of Carbon Capture, Utilization, and Sequestration (CCUS) has gained widespread acceptance as a process involving the capture of CO<sub>2</sub> emissions from industrial processes and fossil fuel power generation. One particularly promising approach involves converting CO<sub>2</sub> into value-added products to diminish its environmental impact. This study focused on a cost-effective, single-step synthesis of a novel nanocomposite consisting of Vanadium and Copper-based layered double hydroxide (VCu LDH) adorned with titanium dioxide nanoparticles (TiO<sub>2</sub> NPs). The synthesized VCu LDH/TiO<sub>2</sub> NPs nanocomposite was assessed for its potential in electrochemically reducing CO<sub>2</sub> in a 0.1 M KHCO<sub>3</sub> solution. Throughout a voltage range of 0.6 to 1.5 V (vs Ag/AgCl), the nanocomposite exhibited the generation of carbon monoxide (CO) and methane (CH<sub>4</sub>) during the electrochemical CO<sub>2</sub> reduction process. Gas products resulting from the CO<sub>2</sub> reduction reaction were analyzed. Notably, C<sub>2</sub>H<sub>4</sub> production was observed between 0.6 and 1.2 V, while a gradual increase in C<sub>2</sub>H<sub>6</sub> formation occurred after 1.2 V. The nanocomposite demonstrated its highest yields of CO, CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>2</sub>H<sub>6</sub> at 1.5 V, 0.8 V, 1.0 V, and 1.5 V, respectively, with amounts of 3394.0, 5710.4, 6307.85, and 4056.33  $\mu\text{mol/t}$  (t=20 mins). These results suggest that the VCu LDH/TiO<sub>2</sub> NPs nanocomposite holds promise as an effective catalyst for CO<sub>2</sub> reduction, with potential applications spanning a wide array of energy conversion and storage contexts.

### Biography

Sneha has expertise in synthesis of novel nanomaterials, electrochemical and photoelectrochemical water electrolysis, seawater electrolysis and electrochemical CO<sub>2</sub> reduction to value added products. Currently, she is working as a Junior Research Fellow on a project funded by Shell Energy India Pvt Ltd and also pursuing her PhD at the Pandit Deendayal Energy University, Gandhinagar, Gujarat, India under the guidance of Dr. Rohit Srivastava. She obtained her degree in B.Sc.-M.Sc. Nano Science & Technology (Integrated) from Shivaji University Kolhapur, Maharashtra, India. She was awarded the SHODH (ScHeme Of Developing High quality research) fellowship by Knowledge Consortium of Gujarat, India.



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## CONTINUOUS PRODUCTION OF A FUNCTIONAL CONSUMER CARE PRODUCT THROUGH PROCESS INNOVATION

Ruaraidh Wells<sup>1</sup>, William Davies<sup>1</sup>, Kevin Bathgate<sup>1</sup> and Xiong-Wei Ni<sup>2</sup>

<sup>1</sup>NiTech Solutions Ltd, UK

<sup>2</sup>Heriot-Watt University, UK

### Abstract:

We will present, for the first time, a real industrial case of converting a batch manufacturing of a functional consumer care product in Croda to continuous production through process innovation. Croda became capacity constrained on a critical batch production asset, the high infrastructure costs of replacing the asset led to the identification of continuous route of manufacturing using NiTech's continuous reactor. The process involves two competing reactions, one leading to the desired product, another being a side product that must strictly be restricted. Mixing and the occurrence of the competing reactions are the main parameters to control. In this presentation, the key problems in batch operations are articulated; the experiences gained and lessons learnt are shared from lab kinetic studies to pilot scale trials with different turn-down ratios and finally to full production. The continuous manufacturing has resulted 99.5% reduction in working mass, 65% reduction in plant footprint, 13-29% per ton reduction in energy utilization, 580 tons per year in CO<sub>2</sub> emission and ~360 MT per year in water saving. These have positively contributed to Croda's ambition of achieving carbon neutral in their manufacturing portfolios by 2030. We hope that this presentation using a real industrial example will simulate interesting discussion, promote innovation and confidence in continuous manufacture of other chemical and pharmaceutical products.

### Biography

Ruaraidh Wells completed his master's degree in chemistry at the University of Glasgow. Since graduating he has gained 5 years' experience in product and process development roles in industrial chemistry. As a Process Development Chemist at NiTech Solutions, Ruaraidh has been involved in R&D project management and execution, as well as client technology transfer projects. Through this experience he has in-depth knowledge in the application of NiTech reactors and crystallizers for material manufacturing within the fine chemical and pharmaceutical sector.

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## AN INVESTIGATION OF SEED MUCILAGE NETWORK PROPERTIES AND ITS FORMATION PROCESS USING COMPUTER MODELLING

**Jacek Siódmiak**

*Bydgoszcz University of Science and Technology, Poland*

### Abstract:

Mucilage, also known as plant hydrogel, is a soft material of significant importance, owing to its biological functions and its potential applications in the development of innovative functional materials. It is odorless, colorless and tasteless substance with emerging commercial potential in agriculture, food, cosmetics and pharmaceuticals due to its non-toxic and biodegradable properties.

In nature, these biomaterials are mainly found in the plant's seed coats. When adequately hydrated, these seed coats exhibit notable properties such as high viscosity and elasticity. The presence of water molecules surrounding macromolecules plays a pivotal role in initiating a range of tribological responses, such as modifying the energy barriers for various intra- and intermolecular interactions. Furthermore, the degree of structural order or disorder is crucial in fulfilling their functions, such as protection and moisture retention. The intricate interactions within the system and their impact on nonlinear viscoelasticity, transport properties, and thermodynamic stability remain areas of limited comprehension.

The primary objective of our research is to elucidate the microrheological properties and structure of mucilage using molecular dynamics (MD). The examined system comprises multiple cellulose fibers encased by pectin molecules, specifically ramnogalacturonan I (RG1) and homogalacturonan (HG), along with hemicellulose, all immersed in an aqueous environment. Our investigation encompasses the study of both intra- and intermolecular interactions within a model plant mucilage system, as well as the diffusion patterns of water molecules in the vicinity of the aforementioned macromolecules. The viscoelastic response of these materials is primarily analyzed through the calculation of mean square displacements of the center of mass of molecules.

### Biography

Jacek Siódmiak's work encompasses various aspects of biophysics. Among the topics he investigates are: non-equilibrium mechanics and statistical thermodynamics, meso- and nanoscale analytical models, and computer simulations of multi-dimensional entropic systems with anomalous kinetics. He also focuses on predicting and controlling fundamental properties of biomaterials with strong amphiphilic characteristics, including colloidal crystals, proteins, and lipid structures. Additionally, his research involves modeling phase transitions such as nucleation and growth of protein and lipid aggregates, which are implicated in various neurodegenerative diseases like Alzheimer's and Parkinson's. Furthermore, he utilizes numerical methods for the analysis of biological signals. He held scholarships at various institutions, including the Central European University, NATO Advanced Study Institute, and CNRS, Laboratory of Theoretical Condensed Matter Physics, Pierre and Marie Curie University.

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## PROMISING QUASI-2D $\text{PDSi}_{2-X}\text{Ge}_X\text{N}_4$ ( $X = 0, 1, 2$ ) CANDIDATE FOR SPONTANEOUS OVERALL WATER SPLITTING

**Radha N Somaiya, and Aftab Alam**

*Indian Institute of Technology - Bombay, India*

### Abstract:

Developing eco-friendly, inexpensive and efficient catalyst for green energy resources has been an ongoing challenge. The successful synthesis of quasi-2D  $\text{MoSi}_2\text{N}_4$  and  $\text{WSi}_2\text{N}_4$  motivated us to investigate three members of this family,  $\text{PdSi}_2\text{N}_4$ , Janus  $\text{PdSiGeN}_4$ , and  $\text{PdGe}_2\text{N}_4$ , possessing excellent stability and promising catalytic performance using density functional theory calculations. These systems acquire appropriate semiconducting electronic band gaps and band edge alignments with robust chemical and dynamical stability. All the three systems are found to self-sustain the photocatalytic mechanism indicating excellent hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) overpotentials.  $\text{PdGe}_2\text{N}_4$  turns out to be the best candidate for HER activity, with a Gibbs free energy ( $\Delta G$ ) as low as  $-0.03$  eV, even better than that of the state-of-the-art Pt catalyst ( $-0.09$  eV). The OER process is spontaneous for all three systems having negative  $\Delta G$  under the influence of potential supplied by photogenerated holes. We strongly believe that the present study will open up further avenues for future experimental studies on these quasi-2D systems.

### Biography

Radha N Somaiya is currently an institute post-doctoral fellow under the mentorship of Prof. Aftab Alam at the Department of Physics at the Indian Institute of Technology Bombay. After completing her master's degree at The Maharaja Sayajirao University of Baroda, she joined the Advanced Materials Lab, under the supervision of Dr. Yogesh Sonvane. Her research interests include computational modelling of materials for energy applications, such as photo(electro)catalysis,  $\text{CO}_2$  reduction,  $\text{N}_2$  reduction and energy storage devices, using ab initio calculations such as DFT and MD simulations. In her thesis, she focused on Silicon based 2D materials for energy and sensing applications. Research findings have been published in well-known international journals in the fields of physics and material science. She has also presented papers at various national/international conferences and workshops in India and received award at an event, including the Best Poster Award at ICRTNCE-2019, SVNIT, Surat, India, EESTER-2018 organized by SRM, SRMIST and IIT Madras, Chennai, India and APS MARCH MEETING 2023 (virtual mode). In addition, she has received a Gold medal for securing first position at master's level. She has pursued her Bachelor of Science degree from Sardar Patel University, Gujarat and secured second position.

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## TURNING CO<sub>2</sub> FROM A LIABILITY INTO AN ASSET WITH THE HELP OF CATALYSIS

Aysel Zahidova<sup>1</sup>, Vahide Mutlu<sup>1</sup>, Özgün Delismail<sup>1</sup>, Eser Hafızoğlu<sup>1</sup>, Başak Tuncer<sup>1</sup> and Erol Şeker<sup>2</sup>

<sup>1</sup>SOCAR Turkey Research & Development and Innovation Inc Aliaga, Turkey

<sup>2</sup>Izmir Institute of Technology, Department of Energy Systems Engineering, Turkey

### Abstract:

New opportunities to use carbon dioxide (CO<sub>2</sub>) in the development of valuable products are capturing the attention of governments, industry and the investment community. Climate change mitigation is the primary driver for this increased interest, but other factors include technology leadership and supporting a circular economy. Innovations like carbon capture and utilization (CCU) and carbon utilization technologies are being explored to reduce emissions while creating useful materials. This could have positive implications for both environmental sustainability and economic growth. Based on reducing its Carbon Footprint for a sustainable world, SOCAR continues important projects in order to transform its own wastes into high value-added fuel/chemicals. The aim to development new catalysts on these area SOCAR R&D carried out catalyst development projects for dimethyl ether (DME) and sustainable jet fuel (SAF) production from CO<sub>2</sub> and hydrogen. This approach showcases how technology and sustainability can intersect to create more eco-friendly solutions for critical sector like aviation.

Within the scope the projects, it is aimed to develop catalysts and processes for the direct conversion of carbon dioxide released into the atmosphere in SOCAR-PETKİM petrochemical production processes into a valuable product- such as dimethyl ether (DME) and SAF.

Within the scope of the project, alumina-based catalysts were synthesized by sol-gel method and tested at a high-pressure reactor at different temperatures by the catalysts group of SOCAR R&D. For DME synthesize the SCR-A named catalysts identified for the synthesis of DME from CO<sub>2</sub> in a single step, and studies are continuing to test the performance of these catalysts in the SOCAR R&D laboratory. For the synthesis of SAF, the identification of candidate catalysts for the conversion of waste carbon dioxide into sustainable aviation fuel (SAF) directly in a single step (in a single catalyst) continues. After the reactions, the gaseous and liquid products were quantitatively analyzed using GC/MS or GC/FID.

### Biography

Aysel Zahidova completed her PhD and MSc at Chemical Engineering Department, Konya Technical University, and Ankara University. She has been studying specifically to develop catalysts for petrochemistry applications. She has experience on synthesize zeolites, nanoparticles, single layer graphenes, modifications of nanoparticles on zeolites, and characterization and testing of catalysts during her master's and PhD. She was involved in the TUBITAK project related to catalysts development for production 2, 6-dimethyl naphthalene from 2-methylnaphthalene. She is working at SOCAR R&D process and catalyst group for 3 years. Today, she is focusing on the project to develop bifunctional catalysts for direct DME synthesis from waste CO<sub>2</sub>.

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## DISCOVERY OF PPAR AGONISTS AS THERAPEUTICS IN METABOLIC DISORDERS

**Iman Ahmed Youssef Ghannam**

*National Research Centre, Dokki, Egypt*

### Abstract:

Hypercholesterolemia and hypertriglyceridemia are two main factors for cardiovascular diseases (CVDs) causing the highest mortality rate worldwide. Peroxisome proliferator-activated receptors (PPAR) isoforms ( $\alpha$ ,  $\gamma$ , and  $\beta/\delta$ ), highly expressed in the liver, heart, kidney, muscles, and adipose tissues, play a crucial regulatory role in lipid metabolism and fatty acid oxidation. Fibrates are PPAR $\alpha$  agonists that are used clinically to reduce cardiovascular diseases burden via improving the blood lipid profiles. Two series of chalcone/quinazolinone fibrate hybrids were designed and synthesized. The synthesized fibrates were tested *in vitro* as PPAR $\alpha$  agonists and their EC<sub>50</sub> values were determined via PPAR $\alpha$  transactivation assay and compared with fenofibrate as a standard. From the *in vitro* experiments, the most active compounds, the synthesized chalcone **10i** and the quinazolinone **9q** fibrate derivatives, were tested *in vivo* for their anti-hyperlipidemic activity using triton-WR 1339-induced hyperlipidemia model in rats. These tested compounds improved the lipid profiles for the treated rats and confirmed by histopathological examinations of the hepatic tissues and found with least toxic effects. PPAR $\gamma$  agonists are responsible for glucose tolerance and insulin sensitivity improvement. A series of novel benzenesulphonamide derivatives were synthesized and tested *in vitro* via PPAR $\gamma$  transactivation assay compared with pioglitazone as a standard. The most active sulphonamide derivatives **9i** and **10d** were then subjected to an immunohistochemical study to study the PPAR $\gamma$  expression in HEPG-2 cells. Furthermore, these compounds were tested *in vivo* for their antidiabetic activity determination using STZ-induced diabetes rat model. The glucose and insulin levels were measured for the treated rats and confirmed with histopathological examination.

### Biography

Ghannam, is associate professor of medicinal chemistry at the Chemistry of Natural and Microbial Products Department - Pharmaceutical and Drug Industries Research Institute - National Research Centre (NRC) - Cairo - Egypt since January 2023. Dr. Ghannam has her area of expertise in the design and synthesis of novel motifs targeting cancer (VEGFR-2 and RAF kinases inhibitors), anti-hyperlipidemia and anti-diabetic therapeutics (PPAR $\alpha/\gamma$  agonists). Dr. Ghannam joined as principal investigator (PI) and Co-PI in several research projects funded from National Research Centre (NRC) and Science Technology Development Fund (STDF) – Egypt [2019-2023] and bilateral co-funded project with Consiglio Nazionale delle Ricerche (CNR) - Italy and NRC – Egypt [2019-2021]. Dr. Ghannam co-supervised M. Sc. and PhD students at the Faculty of Pharmacy Cairo University [2018-2023] and co-authored several publications and reviewed many manuscript in international journals (SCOPUS); European Journal of Medicinal Chemistry, Bioorganic Chemistry Journal, Archiv der Pharmazie Journal and Organic and Biomolecular Chemistry Journal since 2012.



## FLAXSEED OIL EFFECT IN IMPROVING NEUROLOGICAL IMPAIRMENTS IN RAT PUPS INTOXICATED BY ALUMINUM

**Wafaa Lounis**

*University Oran1 ABB, Algeria*

### Abstract:

Aluminum is a very common component of the earth's mineral composition, but it enters the human body in several ways, including drinking water and eating food. Many scientific studies have recently shown that aluminum accumulates in the brain, causing severe neurotoxicity. Given its high amounts of omega 3, flaxseed oil (FSO) might be an important food element and might provide health benefits. 36 young rats (Wistar strain) were collected from a control group and an aluminum chloride-intoxicated females' group (75 mg/kg) for four weeks, the offspring were divided into four groups of 6 rats. Group I (control) served as a control group, and Group II(+FSO) served as a positive control receiving (0.5 mg/kg BW) of FSO issued from control females. Group III (+AlCl<sub>3</sub>) received IP. injection of AlCl<sub>3</sub> (75mg/kg body wt) of group IV (AlCl<sub>3</sub>+FSO) was inoculated by gavage with FSO (0.5 mg/kg body wt) issued from intoxicated females. Neurobehavioral tests were measured by Open Field Test (OFT) and Y-Maze (YMT) Test. The results were processed by one-way ANOVA and TUKEY test. After performing in the OFT arena, the sub-chronic injection of Al chloride to females altered their young rat (group III) locomotor activity and increased the crossing counts in group III. In the YMT data analysis, group III exhibited a smaller number of SAP and more AAR than control rats. This finding suggests that aluminum produces hyperactivity and causes cognitive impairment defined by a lack of short-term memory. The administration of flaxseed oil in group group IV exhibited behavior similar to that of the control group I with a significant difference compared to the AL group. The improvement of dietary FSO on memory and motor hyperactivity in young rats leads to enhance aspects of brain function during conditions of neural disease. The anti-inflammatory properties of omega-3 FA could offer a potential explanation for these results. Neurobehavioral experiments showed significant hyperactivity and memory loss in intoxicated young rats, we suggest that FSO supplementation has neuroprotective effects on developing rat brains.

### Biography

Wafaa LOUNIS, an Algerian who holds a license and a master's degree in Biochemistry and is studying for a doctorate at the same institution (Oran 1 Ahmed Ben Bella University (ABB)), has a strong interest in the domains of neuroscience and neurobehavioral, and reviewer of two renowned, global scientific journals.



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Keynote Presentations



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## GLOBAL GREEN INTEGRATED PROCESS



**Omar Chaalal, Chandra Mouli, Husain Al Hashimi, Marouane Chaalal and Weam Abudaqqa**

*Abu Dhabi University, UAE*

### Abstract:

Carbon dioxide levels in the atmosphere have risen due to massive economic and industrial development around the world. Similarly, the seawater salinity has been increasing for decades as a result of the dumped brine from desalination plants into seas and oceans. The emission of CO<sub>2</sub> has been increasing steadily and with the increasing demand of desalinated water (especially in GCC countries) this is expected to increase at a faster rate. This novel process is using carbon dioxide and rejected brine water to produce green ammonia and green hydrogen as clean fuel for the future.

### Biography

Omar Chaalal is a Professor of Chemical Engineering at Abu Dhabi University. Chaalal has pioneered among others the use of seawater and ammonia to reduce the effect of carbon dioxide on the environment. He has authored 150 refereed publications, 2 European patents, 1 US patent related to smart material in Enhance Oil Recovery and 200 presentations.

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## SYNTHESIS, THEORETICAL AND SPECTRAL CHARACTERIZATION OF BIOLOGICALLY ACTIVE LANTHANIDE(III) COMPLEXES



**Irena Kostova**

*Medical University, Bulgaria*

### Abstract:

Extensive efforts are continually being put into research of complex compounds for medicinal purposes. Lanthanide-based coordination complexes of biologically active ligands have become the source of research and development for potential drug candidates with anticancer and antioxidant activity for last decades.

In the present study a series of bioactive complexes have been synthesized and thoroughly investigated. The physicochemical characterization of the newly obtained lanthanide(III) complexes has been performed using theoretical, spectroscopic and analytical techniques. The computational modelling supported by experimental results can explain the molecular structures, vibrational assignments, reactive sites and structural properties. In this context, to help the binding mode elucidation in the complexes, detailed vibrational analysis was performed on the basis of comparison of experimental (FT-IR, FT-Raman) vibrational spectra of the ligands and Ln(III) complexes with the DFT theory prediction.

The current study was carried out to evaluate the anticancer and antioxidant properties of the Ln(III) complexes. The *in vitro* cytotoxic activity of the studied compounds against cancer cell lines was determined by MTT assay. Taken together the results from the antineoplastic and antioxidant screenings give us reason to conclude that the lanthanide(III) complexes proved to be active cytotoxic and antioxidant agents and strengthen the potential of the complexes as a resource for the discovery of novel anticancer and antioxidant agents.

**Acknowledgments:** The administrative support received by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project No. BG-RRP-2.004-0004-C01 is greatly acknowledged.

### Biography

Irena Kostova is one of the World's Top 1% of scientists according to Stanford University's ranking of scientists with the greatest contribution to the development of modern science. She graduated from Mendeleev University in Moscow with the highest grade. Defended her PhD and DSc theses at MU-Sofia where she is currently a full professor at Chemistry Department. Graduated her second specialization "Theoretical bases of medical chemistry" at MU-Sofia. Her research interests include the developmental work in theoretical and coordination chemistry, vibrational spectroscopy, pharmacological investigations of biologically active compounds etc. Author of about 200 publications with high impact factor and h-index 36, several textbooks, education book materials and monographs with around 7000 citations in indexed journals. She has been a lecturer at renowned universities in India, Austria, Italy, Romania, Spain, Slovakia etc. Member of the organizing committees of over 25 international conferences. She is an Editor of 7 prestigious international scientific journals, a member of the Editorial Boards of over 25 international journals and a reviewer for numerous high-ranking journals and international projects. She has created and maintains collaborations with a number of European universities in the framework of joint research projects and European programs.

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## EXPLORING ENHANCED TWO-DIMENSIONAL ADVANCED ELECTROCATALYST FOR THE PRODUCTION OF GREEN HYDROGEN: APPROACHES TO ACHIEVING CORROSION RESISTANCE IN SEAWATER ELECTROLYSIS



**Rohit Srivastava, and Sneha S Lavate**

*Pandit Deendayal Energy University, India*

### Abstract:

Low-carbon hydrogen deployment is crucial for achieving the Paris Agreement goals and for deep decarbonization of the hard-to-abate sectors (such as heavy-duty transport, steel and fertilizers production, etc.). By the end of 2022, more than 70 countries globally have drafted or already adopted national hydrogen strategies, demonstrating that hydrogen is seen as one of the strategic priorities for the energy sector transition. A burgeoning solution to replace traditional energy sources is the advancement of green hydrogen production through the electrolysis of seawater. This process utilizes renewable sources like solar, wind, and geothermal power to generate green hydrogen, which yields minimal environmentally harmful byproducts. Nonetheless, challenges arise during the seawater electrolysis procedure, specifically concerning the presence of ions like chlorides and sulfates, which induce corrosive issues. The corrosion problem stems from chloride ions infiltrating and oxidizing the metal electrode surface, leading to the release of chlorine gas at the anode. To surmount these obstacles, effective catalysis is crucial for expediting the conversion of water molecules into hydrogen and oxygen. Among catalytic methods, photoelectrocatalysts, a semiconductor-based catalyst, demonstrate promise, with factors such as band gap, charge carrier exchange, and surface area impacting the water-splitting process. Two-dimensional nanomaterials, like layered double hydroxide (LDH), offer advantages like high specific surface areas for electron transfer, tunable functionalities, and flexible structures, rendering them apt for diverse applications. LDH serves as an efficient catalyst for hydrogen production due to its facile synthesis methods, adaptability, and longevity. Additionally, LDH exhibits corrosion inhibition properties through mechanisms like the adsorption of corrosion-related ions, self-healing techniques, and the formation of protective films. This key note talk focuses on the design and development of advanced two-dimensional electrocatalyst for green hydrogen generation and their strategy to deal with sea water electrolysis and also addressing emerging challenges and innovative corrosion mitigation approaches.

### Biography

Rohit Srivastava works as senior Assistant professor in department of petroleum engineering at Pandit Deendayal Energy University (PDEU), India. Prior to joining PDEU, he worked as post-doctoral fellow at Harvard University, United States. At Harvard, he worked with Prof. Juan Perez-Mercader, who was the first director of centro de Astrobiologia (CAB), Spain. His research area focuses on green hydrogen generation, CO<sub>2</sub> reduction into green fuels and origin of life.



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## SYNERGISTIC EFFECT OF N-SUBSTITUTED PYRROLIDINIUM BASED-IONIC LIQUIDS ON AMP: STRATEGY TO COMBAT BACTERIAL RESISTANCE

Juhi Saraswat, Shiv Kumar and Rajan Patel

*Jamai Millia Islamia, India*

### Abstract:

Antibiotic resistance is one of the biggest threats to global health, food security, and development today. Antibiotic resistance occurs naturally, but misuse of antibiotics in humans and animals is accelerating the process. Antibiotic resistance leads to longer hospital stays, higher medical costs and increased mortality. Considerable attention has been directed towards the finding of new alternative antibiotics to counter the bacterial resistance which leads to longer hospital stays, higher medical costs and increased mortality. A suitable solution for these problems is found by using ionic liquids (ILs). ILs have gained considerable global attention due to their diverse applications in various fields of chemical sciences. Since the past few decades, they have attracted significant attention of researchers owing to their unique physicochemical properties such as low vapour pressure, recyclability, non-volatility, and non-combustibility. Though the toxicity of ILs is the most debated topic in their applications as therapeutic agent; several efforts are being made to afford ILs with a balance between their toxicity and application. Therefore, present study involves the synthesis of novel antimicrobial pyrrolidinium based-ILs with varied hydrophobicity that are less-toxic as compared to imidazolium and pyridinium based-ILs. In the present study involves the non-covalent coupling of melittin (MEL), an antimicrobial peptide with a series of synthesized less toxic pyrrolidinium-based ionic liquids (ILs) for which MTT assay was performed. The antibacterial results of conjugates showed remarkable improvement in the MIC value as compared to MEL and ILs alone against *Escherichia coli* and *Staphylococcus aureus*. In addition, hemocompatibility results suggested good selectivity of the non-covalent conjugate as a potential antibiotic agent.



## DETERMINATION OF LEAD IONS ( $\text{Pb}^{2+}$ ) ON SCHIFF BASE LIGAND L-BASED SPCE ELECTRODE IN SEAWATER

**Zahra Akbari, Khoulood Abid, Daniela Iannazzo, Morteza Montazerozohori, and Giovanni Neri**

*University of Messina, Italy*

### Abstract:

Heavy metal pollution is a significant environmental concern due to its adverse effects on ecosystems and human health. Among various heavy metals, lead (Pb) is one of particular concern due to its toxicity, persistence, and bioaccumulation potential. The detection and monitoring of lead ions ( $\text{Pb}^{2+}$ ) in aquatic environments such as seawater are crucial for environmental protection and public health. Electrochemical sensors have emerged as powerful tools for sensitive and selective detection of heavy metals, offering advantages such as rapid response, portability, low cost, and in situ monitoring capability. In this work, a novel bidentate Schiff base ligand is successfully synthesized, (ligand L), through a simple procedure. Herein, we involved the reaction of 1,4-diaminobutane with 2-Methoxycinnamaldehyde in an ethanol solution. The chemical structure of the synthesized Schiff base ligand was thoroughly characterized using Fourier transform infrared (FTIR) spectroscopy, molar conductance measurement and UV-visible spectroscopy. The synthesized Schiff base ligand (L) was further applied for the detection of  $\text{Pb}^{2+}$  in seawater using a screen-printed carbon electrode (SPCE) electrochemical approach in a buffer solution with pH=9. The square wave voltammetry (SWV) technique was employed for the detection process. To enhance the sensitivity of the detection method, gold nanoparticles (AuNps) were utilized to prepare an AuNps-L ligand. This was accomplished through a simple electrodeposition approach, leading to the formation of the AuNps-L complex. Overall, this study demonstrates the successful synthesis of a novel bidentate Schiff base ligand, its characterization using various spectroscopic techniques, and its application for the detection of lead ions in seawater using an electrochemical approach. The incorporation of gold nanoparticles further enhanced the sensitivity of the detection method. These findings contribute to the development of efficient and sensitive methods for heavy metal ion detection in environmental samples.

### Biography

Zahra Akbari, originally from Iran, received her M.Sc. Degree in Inorganic Chemistry from the Department of Chemistry, Shahid Bahonar University, Kerman, Iran, in 2015 and her Ph.D Degree in Inorganic Chemistry from the Department of Chemistry, Yasouj University, Iran, in 2022. She was a visiting researcher for one year with the University of Messina, Italy in 2019, where she joined prof. Giovanni Neri's group and prof. Giuseppe Bruno's group. Her main research activities include the synthesis and characterization of metal complexes and their applications in antimicrobial, antioxidant, and electrochemical sensors. Moreover, she worked in nanomaterial chemistry, focused on nanocatalyst thin films. Currently is a Postdoc researcher at Messina University, Italy.

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## EFFICIENT DATA ACQUISITION OPTIMIZATION FOR CHEMICAL KINETICS: LEVERAGING ORTHOGONAL DECISION TREES AND MACHINE LEARNING

**Grigorii Buklei, and Alexander Tarakanov**

*HSE University, Russia*

### Abstract:

Numerical models play a crucial role in Chemical Engineering, and often these models rely on parameters inferred from experimental data. However, conducting experiments can be both costly and time-consuming. To address this challenge, it is important to design data acquisition processes that extract the maximum information from the measured data. One promising approach to optimize the data acquisition process is through the application of Optimal Bayesian Experimental Design (OBED) techniques. OBED, a method rooted in Mathematical Statistics, quantifies the value of an individual experiment and optimizes the experimental setup to maximize the expected utility of the experiment. Despite its benefits, the direct implementation of OBED can be computationally intensive. In this study, we present a novel approach that leverages a recently developed Machine-Learning algorithm for constructing orthogonal decision trees to accelerate the OBED process. We evaluate the performance of this method through various test cases involving chemical reaction kinetics models. By combining Machine Learning with OBED, we aim to enhance the efficiency and effectiveness of experimental design in Chemical Engineering applications.

### Biography

Grigorii is graduating with a Bachelor's degree in Applied Mathematics and Information Science from Higher School of Economics (Moscow, Russia) in August 2023. Previously, he was a Research Intern at the Complex Systems Modelling and Control Laboratory, Department of Computer Sciences, Higher School of Economics. In November, Grigorii will commence his PhD studies in Mathematics in Natural, Social and Life Sciences at Gran Sasso Science Institute (L'Aquila, Italy). His current research interests encompass mathematical modeling, numerical simulations, and algorithmic game theory. Previously, his work focused on matching theory and the coalitional stability of agents in the context of distributing a common good.



## OPTIMIZATION AND CHARACTERIZATION OF IONIC LIQUID – SURFACTANT BASED NANOEMULSIONS FOR EFFECTIVE PESTICIDE UTILIZATION

**Aashima Anand, Juhi Saraswat, and Rajan Patel**

*Jamai Millia Islamia, India*

### Abstract:

Effective pesticides utilization is a prevailing subject of enormous significance but is often neglected owing the poor solubility or inadequate wettability of the pesticide spray solution. Presently, a water-insoluble insecticide lambda-cyhalothrin (LCT) was selected and loaded into nanoemulsions (NE) prepared with sonication method using a surfactant Tween and two ionic liquids (ILs) each, 1-octyl-1-methylpyrrolidinium bromide [PyrC<sub>12</sub>] Br<sup>-</sup> and 1-dodecyl-1-methylpyrrolidinium bromide [PyrC<sub>12</sub>] Br<sup>-</sup>, in aqueous medium. Different ratios of the surfactant and IL were examined along with varying the magnetic stirring and sonication time and on optimization two NEs were prepared. The effect of the chain length of the IL was also determined. The characterization of these NEs and the NEs loaded with a minimum amount of LCT were done utilizing the techniques of UV-visible spectroscopy and fluorescence spectroscopy. It was found that near the critical micellar concentration (cmc) of the ILs, the formation of the NEs took place. The confirmation of the size and morphology was carried out with dynamic light scattering (DLS) and transition electron microscopy (TEM) and each NE was found to be below 200nm. Further, static contact angle analysis was performed for the prepared NEs (loaded and unloaded with LCT) on the leaves of chili and lemon crops. The NEs were found to enhance the wettability of the insecticide solution. Superior performance was obtained for the long chain IL [PyrC<sub>12</sub>] Br<sup>-</sup>. Moreover, the storage and temperature effect of these NEs was also evaluated with DLS and high stability was established. Hence, the prepared NEs were found to enhance the solubility of the pesticide drastically along with reducing the amount of the same required for its application.

### Biography

Aashima Anand is currently working in the Biophysical Chemistry Laboratory, Jamia Millia Islamia, New Delhi, India, as a Ph.D. Scholar where her main domain is green chemistry. She has her Masters in Applied Chemistry where she had her acquaintance with the various fields of chemistry. She has over 3 years of experience on working with pesticide, surfactants and the green solvents ionic liquids. She has knowledge of extracting and quantifying pesticide residues from crops. She also has sound knowledge of binding interactions involved serum albumins. Also, she has expertise in various analytical techniques such as HPLC, LC-MS, GC-MS, UV-visible spectroscopy, fluorescence spectroscopy, tensiometry, dynamic light scattering (DLS), contact angle analyser. Enhancing the solubility of water insoluble pesticides without the application of harmful organic solvents and overall upgrading the effective pesticide utilization are her chief focus. Through her research work she aims at reducing the use of organic solvents and the quantity of pesticides and thus make the domain of agriculture less dependent on toxic chemicals.

## ASSESSMENT OF NATURAL AND ANTHROPOGENIC CONTRIBUTIONS PARTICULATE MATTER AIR POLLUTION IN DAKAR, SENEGAL

Mamadou Simina DRAME<sup>1,2</sup>, Mame Diarra TOURE<sup>1</sup>, Demba Ndao Niang<sup>1</sup>, Thierno DOUMBIA<sup>3</sup>, Kharouna TALLA<sup>1</sup>

<sup>1</sup>FST/Département de Physique/Université Cheikh Anta Diop de Dakar, Sénégal

<sup>2</sup>Laboratoire de Physique de l'Atmosphère et de l'Océan Siméon Fongang, Université Cheikh Anta Diop, Sénégal

<sup>3</sup>Laboratoire d'Aérodologie, CNRS, France

### Abstract:

This study investigates air pollution levels, specifically particulate matter (PM<sub>10</sub> and PM<sub>2.5</sub>), in Dakar, West Africa, due to its significance as a major public health concern. The region is notable for being a substantial contributor to global desert dust, compounded by high levels of air pollutants from human activities. Data from the Air Quality Management Centre (CGQA) between 2010 and 2015 at five Dakar stations were utilized. The preliminary findings highlight alarmingly elevated levels of PM<sub>10</sub> and PM<sub>2.5</sub>. Annual average PM<sub>10</sub> concentrations in Dakar surpass the WHO recommended limit by over 7.2 times, and the Senegalese recommended limit by 1.8 times. Although Senegal lacks a PM<sub>2.5</sub> thresholds, its pollution level exceeds WHO guidelines by 3.7 times. A pronounced seasonal cycle is also observed, with peak concentrations during the dry season (December to May) and troughs during the wet season (June to November). To evaluate anthropogenic pollution attributed to traffic and industry in Dakar, we focused on the weekly distribution of PM<sub>2.5</sub> concentrations between 2010 and 2015. In contrast to weekdays, the minimum PM<sub>2.5</sub> concentrations (around 31 µg/m<sup>3</sup>) are recorded on Sundays when human activities are least intense. This minimum value represents a baseline PM<sub>2.5</sub> concentrations consistently present in Dakar's atmosphere. Overall, anthropogenic contributions of PM<sub>2.5</sub> range between 5 and 7 µg/m<sup>3</sup> on a daily basis. Lastly, the hourly distribution (diurnal cycle) of PM<sub>2.5</sub> substantiates this contribution, with levels ranging from 5 to 7 µg/m<sup>3</sup>, fluctuating from pre-activity morning hours to the peak of anthropogenic activities during the day.

## ANTIOXIDANT PROPERTIES OF A NOVEL TRIAZOLE LIGAND AND ITS LANTHANIDE(III) COMPLEXES

**Lozan Todorov, Nadya Hristova-Avakumova, Nataliya Belskaya and Irena Kostova**

*Medical University, Bulgaria*

### Abstract:

Lanthanides and their chemical compounds are an essential building block of modern advanced technology. Their applications are ubiquitous – in lasers, industrial magnets, thermonuclear reactors, photocatalytic systems, electric cars, solar cells, anti-counterfeit protection of banknotes, wind turbines, NMR contrasts, etc. to name just a few. Their utility is based to a large extent on the excellent fluorescent properties of lanthanide atoms and ions as well as their intrinsic magnetism. Serious efforts have been invested into research of novel lanthanide applications in biology, medicine and pharmacy with varying degrees of success so far. Their excellent fluorescent properties and ionic mimicry towards a number of biometals, combined with the so-called fluorescent ligand “antenna effect” make lanthanide complexes suitable candidates for novel theragnostic agents. 1,2,3-Triazole is a very prominent pharmacophore, a component of a large number of medicinal molecules – anticancer, antimicrobial, antidiabetic, neuroprotective, etc. The present study elucidates the potential antioxidant biological activity of a fluorescent 2*H*-1,2,3-triazole-bearing ligand (BNP02 - Sodium 2-(4-methoxyphenyl)-5-(pyrrolidine-1-yl)-2*H*-1,2,3-triazole-4-carboxylate)) and its complexes with lanthanide(III) ions ( $\text{Ln}^{3+}$ ). The ligand and its  $\text{Ln}^{3+}$  complexes were tested for scavenging activities against a multitude of biologically significant reactive species – hydroxyl radicals, generated by UV-induced water radiolysis and Fenton reaction; superoxide, derived from potassium superoxide and xanthine/xanthine oxidase enzymatic model system; hypochlorite, derived from sodium hypochlorite. In addition, possible mechanisms of radical scavenging were investigated by way of the DPPH and ABTS assays. UV-VIS spectroscopic and chemiluminometry studies were applied. Relative differences between the activities of the various complexes were observed and described and the impact of the coordination center i.e., type of  $\text{Ln}^{3+}$  ion on antioxidant activity was revealed.

### Biography

Lozan Todorov currently serves as a Senior Assistant Professor at the Department of Chemistry at the Faculty of Pharmacy in Medical University – Sofia, Bulgaria. His PhD thesis, under the scientific supervision of prof. Irena Kostova, deals with antioxidant properties of gallium and lanthanum complexes with 5-aminoorotic acid. He has participated in and overseen a number of university-level projects in close collaboration with Dr Hristova-Avakoumova at the Department of Medical Physics and Biophysics at the Faculty of Medicine, Medical University-Sofia. Dr Todorov's research experience includes a variety of antioxidant assays, involving a different reactive species, derived from various model systems. His current research interests are associated with the promising field of lanthanide coordination chemistry and its potential applications in biomedical sciences. To that effect, together with prof. Kostova, Dr Hristova-Avakoumova and in collaboration with a multinational research team, including prominent scientists from Spain, India and Italy, Dr Todorov is participating in a new project “Biologically Active Heterocyclic Ligands and Metal Complexes with Antioxidant Activity”, part of the Research Universities program, financed by the European Union, the Bulgarian Ministry of Education and the Bulgarian National Sciences Fund.

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## COPPER-MODIFIED HETEROATOMIC CE-MWW ZEOLITES AS POTENTIAL NO CONVERSION CATALYSTS

**Aleksandra Jankowska, Klaudia Fidowicz, Andrzej Kowalczyk, and Lucjan Chmielarz**

*Jagiellonian University, Poland*

### Abstract:

Zeolites are known catalysts and carriers of the catalytically active phase, commercially used in many branches of the chemical industry. One of the representatives of zeolites of synthetic origin is MCM-22, belonging to the MWW family. In this study, a modification of the layered MCM-22 zeolite precursor was carried out, taking into account modifications of the structure, including the introduction of heteroatoms (Ce), obtaining micro-mesoporous derivatives (ITQ-2 and MCM-36), as well as catalytic activation of precursors with copper cations. The structure of each material was modified with Ce (Si/Ce=30). Cerium has a high redox and oxygen storage capacity, which increases the material's acidity and provides active oxygen species to oxidize NO to reactive NO<sub>2</sub>. The formation of NO<sub>2</sub> is necessary for the activation of low-temperature NO<sub>x</sub> conversion according to the fast-SCR mechanism. The obtained materials were found to be active and selective catalysts for use in the low-temperature NO conversion process, especially below 250°C, which makes them potential catalysts for use in low-dust NH<sub>3</sub>-SCR stationary installations.

### Biography

Aleksandra Jankowska graduated her PhD at the Jagiellonian University in Kraków (Poland) in 2023. Research for her PhD thesis is being realised in the Environmental Technology Research Group, which is a part of the Chemical Technology Department. Her scientific interests are related to the synthesis, modification and functionalization of modern porous silica materials, including zeolites and mesoporous silica sieves, for their application in the conversion of gaseous nitrogen pollutants (NH<sub>3</sub>-SCR, selective catalytic reduction of NO<sub>x</sub> with ammonia). She is the Principal Investigator of the Preludium 20 project funded by the National Science Centre of Poland.



Day 2

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Poster Presentations

## THE POTENTIAL FOR UTILIZING SLUDGE FROM THE KENITRA WASTEWATER TREATMENT PLANT IN AGRICULTURAL PRACTICES

Noura Benlemlih<sup>1</sup>, Safae EL AAMMOURI<sup>1</sup>, Ali HAMMANI<sup>2</sup> and Mohamed IBRIZ<sup>1</sup>

<sup>1</sup>University of Ibn Tofail, Morocco

<sup>2</sup>Institut Hassan II d'Agronomie et de Médecine, Morocco

### Abstract:

The Régie Autonome de Kénitra (RAK) has adopted the vision of using dewatered sludge in agriculture, provided that it meets the requirements. To this end, we studied the feasibility of this valorization during the three months of our internship. The physico-chemical parameters studied were : Dry matter (DM), volatile dry matter (VDD), pH, dryness, fertilizing elements and heavy metals.

The average values of the sludge physico-chemical analyses are as follows: MS (31.11g/l); MSV (16.77g/l), pH (8.11), dryness (22.36%): TKN (46 mg/kg), total phosphorus (733 mg/kg), potassium (159.75 mg/kg).

Heavy metal analysis revealed that the sludge's heavy metal content complied with application standards (Cd 0.22 mg/kg MS, Cr 106.27 mg/kg MS, Cu 37.48 mg/Kg MS, Hg 1.33 mg/Kg MS, Ni 7.66 mg/Kg MS, Pb 12.75 mg/Kg MS).

It can be said that the sewage sludge from the Kenitra WWTP is of real agronomic interest, as it is rich in fertilizing elements, but in the absence of a microbiological analysis of this sludge, it is impossible to make a decision concerning its use in agriculture. Consequently, the research carried out requires further investigation to confirm the feasibility of recovery from green manures and the reduction of specific pollution.

### Biography

Noura BENLEMLIH , 39 years old , PhD student researcher in 2nd year affiliated to the Laboratory of vegetal, Animal Productions and agro-industry, Faculty of Science, University of Ibn Tofail , B.P 242 Kenitra 14000, Morocco with 2 scientific publications indexed SCOPUS Holder of a Master degree in Biology of the environment , bachelor's degree in applied microbiological life sciences and molecular biology of the cell , bachelor's degree in life sciences , chemical physics degree and a Bachelor degree in Life and Earth Sciences in 2002.



## EFFECTIVE CATALYSTS FOR LOW-TEMPERATURE NH<sub>3</sub>-SCR PROCESS BASED ON COPPER-MODIFIED MCM-41 MESOPOROUS SILICA – COMPARISON OF TIE AND ADP METHODS

Aleksandra Gomulka<sup>1</sup>, Andrzej Kowalczyk<sup>1</sup>, Zofia Piwowarska<sup>1</sup>, Lucjan Chmielarz<sup>1</sup> and Pegie Cool<sup>2</sup>

<sup>1</sup>Jagiellonian University, Poland

<sup>2</sup>University of Antwerp, Belgium

### Abstract:

Mesoporous silica materials show excellent potential in catalysis because of several unique properties, such as homogeneous porous structure, very large specific surface area and porosity. However, mesoporous silicas do not naturally exhibit an ion-exchange ability, which could facilitate their functionalization. Consequently, the process of depositing catalytically active components in highly dispersed and uniform form is both intricate and costly, which significantly limits using such materials on a wider scale. For this reason, to deposit copper on the surface of mesoporous silicas in a homogeneous form, two very interesting methods of modification were used – template ion exchange method developed with ammonia treatment (TIE-NH<sub>3</sub>) and ammonium driven deposition precipitation method (ADP). In both TIE and ADP methods, copper salts were used as precursors of the active phase and ammonia as reactant supporting its high dispersion. However, the mechanism of copper deposition using ADP method significantly differs from the TIE process. On the one hand, TIE method is based on exchange of cationic surfactants in freshly prepared samples of mesoporous silica (non-calcined) for metal cations. Directly after TIE procedure samples are treated with ammonia solution, which provides high dispersion of deposited copper species. On the other hand, in ADP method, after ammonia addition to a solution containing copper ions, ammonia coordinates copper cations forming distorted octahedral cationic species. Due to its positive charge, such ammonia coordinated copper cations undergo electrostatic adsorption on the surface of mesoporous silicates when hydroxyl groups are deprotonated and present in the Si-O<sup>-</sup> form. ADP method is used for deposition of copper species on calcined mesoporous silica materials. Unfortunately, ammonia used in both methods can cause partial destruction of the ordered porous structure of MCM-41 silicas. For this reason, the study aimed to compare the effectiveness of copper deposition on the surface of mesoporous supports, including the influence of ammonia on silica porous structure destruction, were carried out. MCM-41 silica material modified with copper deposited in a highly dispersed form were found to be a very promising catalytic system for the low-temperature NH<sub>3</sub>-SCR process.

### Biography

Aleksandra Gomulka started her doctoral studies at Faculty of Chemistry of Jagiellonian University in 2021. She carries out her research work in Environmental Technology Research Group under scientific supervision of prof. Lucjan Chmielarz. Her research work is focused on the synthesis of high surface porous materials of MCM-41 and MCM-48 types and their functionalization with transition metals to obtain effective catalysts for important environmental processes, such as Selective Catalytic Reduction of nitrogen oxides, NO<sub>x</sub>, with ammonia (NH<sub>3</sub>-SCR) and Selective Catalytic Oxidation of ammonia (NH<sub>3</sub>-SCO). The starting point in her research is deposition of selected transition metals on mesoporous silicas of the MCM-41 and MCM-48 types by template ion-exchange (TIE) method. The high dispersion of deposited metal species can be controlled by treatment of the samples directly after TIE procedure with ammonia solution (e.g., in the case of copper species deposition). This modified version of TIE method was developed in Environmental Technology Research Group. Unfortunately, the side effect of ammonia treatment is a partial

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destruction of the ordered porous structure of mesoporous silicas. One of the main goals of her studies is development of alternative to ammonia complexing agents with a similar efficiency in protection of highly deposited transition metals species, but less reactive in degradation of porous structure of mesoporous silica materials. At the second year of doctoral studies, she completed a five-weeks research internship at University of Antwerp (Belgium) in the research group headed by prof. Pegie Cool. During the internship she got acquainted with ADP method and obtained catalysts based on MCM-41 and MCM- 48.

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## WASTEWATER TREATMENT BY INFILTRATION PERCOLATION PROCESS USING FINE SAND AND ACTIVATED CARBON

**Safae EL AAMMOURI, Noura BENLEMLIH and Mohamed IBRIZ**

*University of Ibn Tofail, Morocco*

### Abstract:

The aim of this study was to find a cost-effective wastewater treatment system for use in disadvantaged regions and countries. To this end, two filtration systems were implemented to treat wastewater from a wastewater treatment plant in Morocco. The first system is an intermittent sand filter (ISF) using fine sand, while the second is a modified infiltration percolation (MIP) based on activated carbon.

Before and after the water passed through the filters, physico-chemical and bacteriological analyses were carried out. The results showed a significant reduction in physico-chemical parameters such as suspended solids (SS), with an abatement rate of 99.6% for ISF and 99.4% for MIP. Similarly, chemical oxygen demand (COD) was reduced by 17.7% for ISF and 55% for MIP. As for biochemical oxygen demand (BOD5), the ISF showed a reduction of 7.14%, while the MIP was much more effective, with a reduction of 100%.

Although both filters succeeded in considerably reducing the concentration of faecal coliforms, with respective abatement rates of 98.2% for ISF and 99% for MIP, the final concentration of these bacteria remains above regulatory standards.

### Biography

Safae EL AAMMOURI, 28 years old, PhD student researcher in 2<sup>th</sup> year affiliated to the Laboratory of vegetal, Animal Productions and agro-industry, Faculty of Science, University of Ibn Tofail, B.P 242 Kenitra 14000, Morocco with 2 scientific publications indexed SCOPUS Holder of a Master degree in Engineering of Natural Resources Valorization and Quality Management in 2019, a Bachelor degree in Sciences and Techniques water and environmental engineering and a Bachelor degree in Life and Earth Sciences in 2012.

## THE EFFECT OF IRON ADDITION IN SILICA-TITANIA MESOPOROUS CATALYSTS ON THE EFFICIENCY OF THE DIPHENYL SULFIDE OXIDATION PROCESS

Wiktoria Dubiel<sup>1</sup>, Andrzej Kowalczyk<sup>1</sup>, Marek Michalik<sup>1</sup>, Włodzimierz Mozgawa<sup>2</sup>, Marcin Kobielusz<sup>1</sup>, Wojciech Macyk<sup>1</sup>, Lucjan Chmielarz<sup>1</sup>

<sup>1</sup>Jagiellonian University, Poland

<sup>2</sup>AGH University of Science and Technology, Poland

### Abstract:

Development of a highly efficient catalytic process for the production of organic sulfoxides and sulfones is the goal of many research works due to the importance of these reagents. One of the objects of interest is diphenyl sulfide and products of its oxidation. Diphenyl sulfoxide is a significant chemical used as intermediates in various organic synthesis, enzyme activator as well as a metal extraction agent, while diphenyl sulfone is used in chemical, pharmaceutical, agrochemical, polymer or plastic industry. The formation of sulfoxides and sulfones from their corresponding sulfides is usually achieved by using stoichiometric quantities of corrosive oxidizing agents, such as oxone, manganese, peracid and nitrate. The alternative, more environmental-benign method, is using hydrogen peroxide as an oxidant. In such a case, the process requires catalytic or photocatalytic conditions, however it can be performed in mild reaction conditions as room temperature and atmospheric pressure.

In our previous studies, spherical, mesoporous silicas, obtained by co-condensation, containing titanium in the structure (Ti-S-MCM-41) were tested as catalysts and photocatalysts of diphenyl sulphide oxidation to diphenyl sulfoxide and sulfone in the presence of H<sub>2</sub>O<sub>2</sub>. The promising results of these studies initiated the extension of the material series to include bimetallic samples, modified with titanium and iron. An analogous synthesis of materials was carried out using the co-condensation method. Samples were characterized in terms of chemical composition (ICP-OES), structure and morphology (XRD, SEM), textural parameters (low-temperature N<sub>2</sub> sorption), metal form and aggregation (UV-Vis-DRS, Raman). It was found that the addition of iron into Ti-mesoporous silicas makes the aforementioned reaction more efficient than for the reference sample, modified only with titanium.

### Biography

Wiktoria Dubiel is PhD student at the Doctoral School of Exact and Natural Sciences in the chemical sciences program at Jagiellonian University in Kraków, Poland. She is a member of the Environmental Technology Research Group. She started working in this research team during her undergraduate studies. She is graduated with honors and a high grade point average, defending her master's thesis entitled: "Modern zeolite materials of the SiO<sub>2</sub>@ZSM-5 type as catalysts for dimethyl ether synthesis". In the second year of her doctoral studies, she completed two international scientific internships in highly reputable research institutions, VSB - Technical University of Ostrava (Czech Republic) and Instituto de Tecnología Química (Valencia, Spain). Completed internships, conducted research and learned innovative techniques of syntheses and catalytic processes significantly enriched her scientific experience. Her current research focuses on the synthesis and functionalization of porous silica-titania materials as catalysts and photocatalysts for the process of selective diphenyl sulphide oxidation in the presence of hydrogen peroxide as an oxidant, which is the subject of her doctoral thesis.

## PROPHYLACTIC ROLE OF CAFEIC ACID AGAINST ALUMINUM-INDUCED KIDNEY DAMAGE IN WISTAR RATS

**Chouari Zehor, Kessas Khadidja, Lounis Wafaa and Kharoubi Omar**

*University of Oran1ABB, Algeria*

### Abstract:

**Objective:** Aluminum (Al) poisoning has attracted considerable interest, as it is almost impossible to avoid exposure to this metal, as it is used in various daily applications. Antioxidants and phenolic compounds have often been considered as chemoprotective agents to regulate the progression of diseases related to the production of reactive oxygen species. The aim of this work is to study the effect of caffeic acid (CA) on Al-induced weight gain and renal dysfunction.

**Material and methods:** In this study, 40 male Wistars rats weighing  $70 \pm 10$  g are divided into 4 groups: Group 01: control rats which received no treatment; Group 2: rats poisoned by an intraperitoneal injection of 60mg/kg of Al; Group 3: rats poisoned by an intraperitoneal injection of 60 mg/kg of Al and treated with 30mg/kg of CA by gavage and a 4th group: the rats are treated only with CA (30mg/kg by gavage) for 45 days, the rats were weighed daily. At the end of the experiment, the rats are sacrificed, the blood is taken and the kidneys are homogenized then centrifuged, the supernatant thus obtained is used for the evaluation of the biochemical parameters.

**Results:** Our results show that Al causes a significant decrease in body weight and kidney weight, with a significantly lower relative weight in the intoxicated group compared to the control group; and negatively affects renal function by increasing the serum level of uric acid and creatinine, as well as increasing the level of TBARS at the tissue level in addicts compared to controls. On the other hand, treatment with caffeic acid showed a protective effect on the kidneys, by increasing body weight and correcting the content of creatinine, uric acid and lipid peroxidation products.

**Conclusion:** The present work demonstrated that caffeic acid has the ability to protect against aluminum-induced renal dysfunction and oxidative stress.

### Biography

Zehor Chouari was born in Oran, Algeria, in 1995. She obtained her "Licence" at Oran 1 Ahmed Ben Bella University (ABB), in 2017 specializing in Biochemistry, then she obtained her "Master" in Biochemistry specialty in 2019. Currently, she is pursuing her doctorate in the Department of Biology, specialty "Applied Biochemistry" of the same university. His areas of research are toxicology and liver damage induced by oxidative stress.

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## EVALUATION OF BLUEBERRY POMACE FOR THE PRODUCTION OF ANTIOXIDANT COMPOUNDS THROUGH ENRICHED NATURAL FERMENTATION

**Vivian García Rojas, Karina Stucken; Claudia Godoy, Angela Rodriguez and Jocelyn Cortes**

*Universidad de La Serena, Chile*

### Abstract:

Currently, healthy, natural and health-beneficial foods are being preferred by the world's population, with berries being a market of great interest to the consumer public. A relevant part of blueberry production is destined for processing such as juices or wines, resulting in approximately 20% of by-product, waste or residue, which consists of solid waste that is generated mainly from the skins and seeds of the fruits, called cranberry pomace, which is wasted and is a source of bioactive compounds that are wasted. Enriched natural fermentation refers to a lactic fermentation process where the sugars present in a food are converted into lactic acid through the use of facultative anaerobic lactobacteria native or native to the matrix, thus allowing the release of other compounds present in the food. the food matrix. Therefore, this study determined the effects of enriched natural fermentation on the bioactive composition of blueberry pomace, studying the change in the phenol profile, the content of total polyphenols. Selective natural fermentation was carried out with microorganisms obtained from fresh blueberries and fermented for 15 days. The results show an increase in the ac content. gallic from a non-detectable level to 141 mg/100 g m.s. on day 13 of fermentation, ac. Protocatechuic showed a peak increase on day 8 of fermentation and quercetin increased from a non-detectable level to 196.3 mg/100 g m.s. on day 15 of fermentation. Regarding the content of total polyphenols, an increase of 23.89% was obtained on day 15 of fermentation compared to the initial content. Concluding, the application of enriched natural fermentation improves the release and/or transformation of bioactive compounds in blueberry pomace.

### Biography

Vivian García is a food engineer of University La Serena in 2018 and doctoral student in food and bioprocess engineering, University of La Serena in Chile, her lines of research are Food Microbiology and Fermentation of food matrices, Functional foods and biocompounds, Dehydration process engineering and Biomaterials. She currently working on her doctoral thesis whose title is: "Stabilization of sulforaphane-rich extracts and bioactive compounds from fermented broccoli in Pickering emulsions." She have participated in research and product development projects, in addition to financing our dissemination through fairs and scientific forums like as 1)Make It ULS Project No. MIT229, titled "Encapsulating substances of high biological interest for health.", 2) CIV-VAL Node: Thesis to impact the territory 2023, and 3)Apply your idea, Copec-UC Foundation. Her Participation in Fairs: Third version of the Make It Fair and forum: Future solutions for the territory. Recognized in the "Innovative Student" category of the Crea e Innova event organized by the Research and Development Directorate of the University of La Serena, for innovative proposals for the revaluation of broccoli discards.





Day 2

**Chemistry  
Congress  
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Catalysis 2023**

Video Presentation

## THE VITAMIN D, IL-6 AND THE eGFR MARKERS A POSSIBLE WAY TO ELUCIDATE THE LUNG-HEART-KIDNEY CROSS-TALK IN COVID-19 DISEASE: A FOREGONE CONCLUSION

**Diego Tomassone**

*"Holos Medica" Clinical and Research, Italy*

### Abstract:

Based on recent findings, we speculated the existence of the lung, heart, and kidney axis as the main pathway for the COVID-19 disease progression. Methods: This paper reports on an observational study conducted by a team of researchers and doctors of the 118-Pre-Hospital and Emergency Department of SG Moscati of Taranto City in Italy. The study was conducted on a totality of 185 participants that were divided into three groups. The study group included COVID-19 affected patients (PP n = 80), the first control group included patients with different pathologies (non-COVID-19 NNp n = 62) of the SG Moscati Hospital, and the second control group included healthy individuals (NNh n = 43). The core of the current trial was focused on assessing the level of the vitamin D (serum 25(OH) D concentration), IL-6, and the renal glomerular filtrate (eGFR) in COVID-19 disease and non-COVID-19 patients in both groups. Results: It was observed that the majority of COVID-19-infected patients showed a progressive multi-organ involvement, especially in regard to the lung, kidney, and heart. The majority of the COVID-19 patients exhibited preexisting comorbidities which include cardiovascular, respiratory, and renal disorders accompanied by a severely low level of vitamin D, extremely high level of IL-6, and low glomerular filtration rate (eGFR). The significant overall damages exerted by the immune-mediated responses under the hyper-expression of proinflammatory cytokines and interleukins, such as IL-6, may be facilitated by either a decreased level of vitamin D or the ageing process. The reduced presence of vitamin D was often found together with a reduced functionality of renal activity, as revealed by the low eGFR, and both were seen to be concomitant with an increased mortality risk in patients with lung disorders and heart failure (HF), whether it is showed at baseline or it develops during manifestation of COVID-19. Therefore, the documentation of the modifiable risk factors related to SARS-CoV-2 and lung impairment in older patients with kidney and heart disease may help the clinician to better manage the situation. Conclusions: This paper addresses how a low level of vitamin D and older age may be indicative of systemic worsening in patients with COVID-19, with a goal of providing a broader context in which to view a better therapeutic approach. From this presentation, taken from the work published in 2021 by the research group of which I was a member, it will be possible to learn the importance of evaluating parameters such as the dosage of Vitamin D, a hormone and fundamental immunomodulant in our body, both to prevent and to treat through supplementation, infectious diseases such as Covid-19.

### Biography

Diego Tomassone received master's degrees in Medicine, Chemistry and Physics, a bachelor's degree in Mathematics and a Ph.D. in Infectious Diseases, Microbiology and Public Health. He directs the medical center "Holos Medica" clinical and research, working as a clinical physician and researcher, also dealing with research in physics and chemistry. He has published about 20 papers on Covid-19 disease alone, co-author of Chapter 12 of the scientific paper: "COVID-19 infection as a chronic disease: Factors and pharmacological perspectives". He is also FoPRC (Foundation of Physics Research Center) researcher, reviewer and editorial board member of several international scientific journals.

## FERMENTATION WITH NATIVE MICROORGANISMS IN RAW, BLEACHED AND STERILIZED BROCCOLI PUREE AS A STRATEGY TO INCREASE THE SULFORAPHANE CONTENT

Vivian García Rojas, Karina Stucken and Jocelyn Cortes

*Universidad de La Serena, Chile*

### Abstract:

**Objective:** Apply to the fermentation with native microorganisms in broccoli puree demonstrating that fermentation is a viable strategy to produce SFN a compound of high biological interest.

### Methods:

**Broccoli puree:** Three pre-treatments were considered for the inflorescences: Raw broccoli, Sterilized broccoli sterilized at 121°C for 15 min and blanching broccoli in a thermoregulated bath at 57°C for 13 min. all samples was brought to a in a 1:3 ratio with sterilized water for puree formulation.

**Starter cultures:** A broccoli floret is taken and incubated at 37°C in MRS broth, to previgilate growth of lacto-bacteria, later glyceric, obtaining our stock culture.

**Brocoli puree fermentation:** each broccoli puree was inculted with the starter culture at a concentration of 108 CFU, fermentation was carried out in a shaker at temperature at 35°C for 20 day.

**Sulforaphane content:** SFN was quantified in reverse phase HPLC according to Mahn et al., 2020.

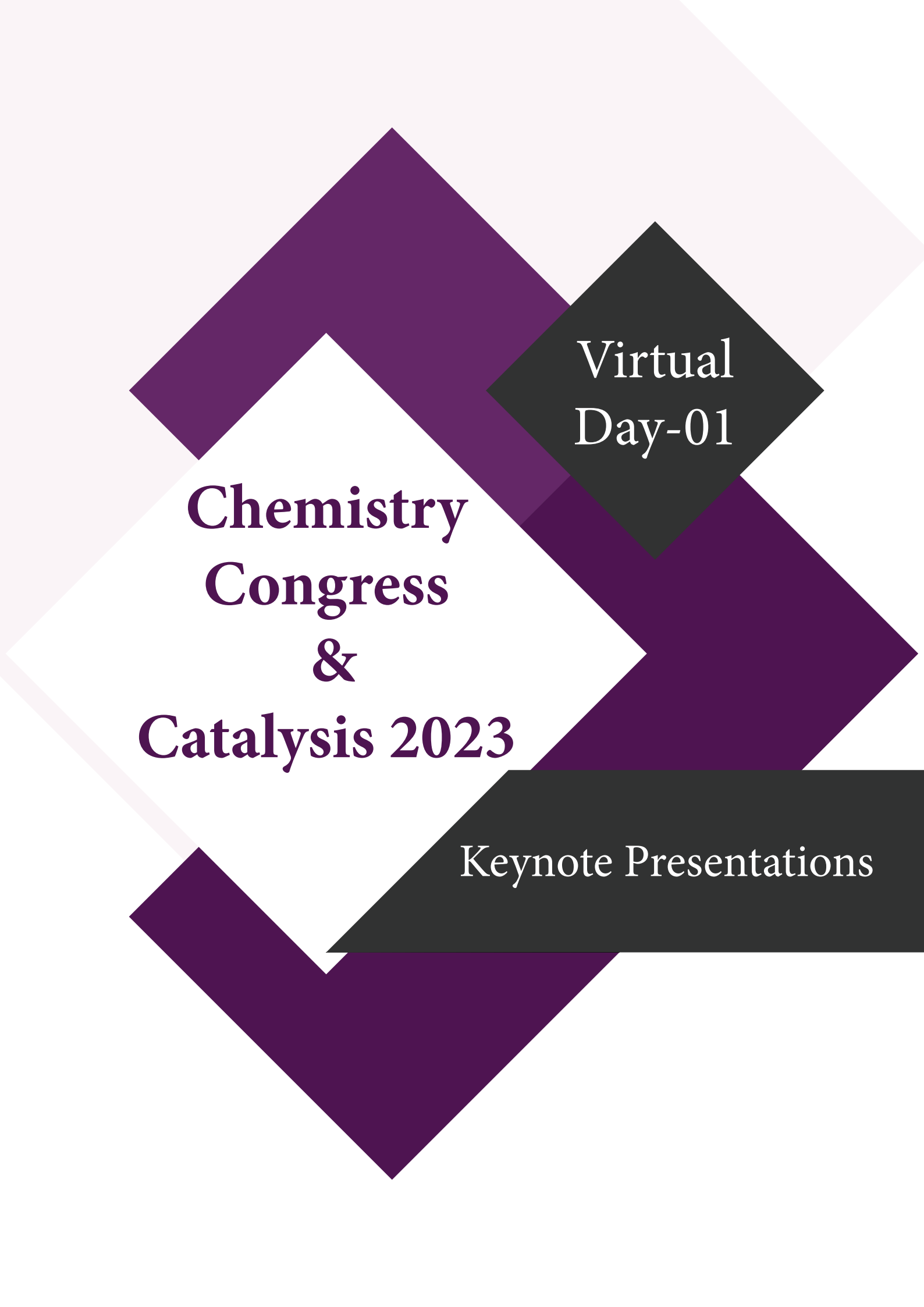
**Results:** The SFN in all cases showed an increase because of fermentation, raw SFN without fermentation is  $1.15 \pm 0.02$  mg SFN/g m.s, increasing to  $6.50 \pm 0.54$ ,  $9.74 \pm 0.33$  and 467.91 mg SFN/g m.s. puree sterilized, raw, and bleached respectively. all the fermentations were showing a tendency to increase the SFN content, but at different times of sampling.

**Conclusion:** Fermentation with native microorganisms increases the SFN content, showing better results in blanched broccoli puree. This may be due to the inactivation of enzymes that divert the SFN synthesis towards other degradation compounds. In addition, the bleaching conditions allow myrosinase to remain active endogenous broccoli

### Biography

Vivian García is a food engineer of University La Serena in 2018 and doctoral student in food and bioprocess engineering, University of La Serena in Chile, her lines of research are Food Microbiology and Fermentation of food matrices, Functional foods and biocompounds, Dehydration process engineering and Biomaterials. She currently working on her doctoral thesis whose title is: "Stabilization of sulforaphane-rich extracts and bioactive compounds from fermented broccoli in Pickering emulsions." She have participated in research and product development projects, in addition to financing our dissemination through fairs and scientific forums like as 1)Make It ULS Project No. MIT229, titled "Encapsulating substances of high biological interest for health.", 2) CIV-VAL Node: Thesis to impact the territory 2023, and 3)Apply your idea, Copec-UC Foundation. Her Participation in Fairs: Third version of the Make It Fair and forum: Future solutions for the territory. Recognized in the "Innovative Student" category of the Crea e Innova event organized by the Research and Development Directorate of the University of La Serena, for innovative proposals for the revaluation of broccoli discards.

# **Virtual Presentations**



Virtual  
Day-01

**Chemistry  
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Keynote Presentations

## PLASTIC TRASH TO MONOMERS AND INTERMEDIATES – PTMI

**Anne M. Gaffney**

*University of South Carolina, USA*

### Abstract:

To address the issue of waste plastics in landfills, a hybrid approach is proposed. This would use low temperature plasma pretreatment followed by catalytic cracking to augment the conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals. Lightweight packaging (LWP) comprises about 50% of total plastics consumption and consists mainly of single and multilayer films and containers. LWP is heterogeneous, contaminated and is difficult to recycle. Mechanical recycling is currently the only commercial approach to recycling but is inadequate to address the growing volume of packaging plastics and degrades or downcycles both polyethylene (PE) and polypropylene (PP). In contrast, feedstock recycling converts polymers to monomer feedstock that can be used to make new products that have virgin-like performance in high volume single use packaging applications, thereby creating new value chains for what is currently a waste stream. Current high TRL feedstock recycling technologies like pyrolysis and gasification are highly energy intensive, require multiple steps (plastics-syngas-methanol-olefins) and have low selectivity to polyolefin building blocks (ethylene, propylene). Alternatively, plastics upcycling aims at selectively deconstructing polymer in a one-step process directly into monomers and high value chemicals (HVC). Consequently, it is proposed to use a hybrid approach of preconditioning with a low temperature plasma followed by catalytic cracking for conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals. This offers improvement in carbon utilization, cumulative energy demand and selectivity to recycled high value products over current benchmark feedstock recycling processes like gasification and pyrolysis. It is suggested to use LTP treatment as a tunable polyolefin functionalization step to increase selectivity of subsequent catalytic deconstruction and reconstruction. The target waste stream is post-industrial and post-consumer packaging waste, mainly LDPE, LLDPE, and PP films. The primary target products from this novel process are C<sub>2</sub>-C<sub>4</sub> olefins (ethylene, propylene, butylene) which are the raw materials for bulk of the volume of single use plastic production (PE and PP). Aromatic and other HVC precursors like benzene, toluene, xylene (BTX), ethyl benzene and polyols are also expected as by-products from the process. All the products and by-products (C<sub>2</sub>-C<sub>4</sub> olefins, BTX, polyols, HVC) can be upcycled to resins, bulk (polyethylene, polypropylene) and specialty polymers (polyurethanes, epoxy, polyester, Nylon-6) at different market entry points.

### Biography

Anne M. Gaffney is the Chief Science Officer of Idaho National Laboratory and Distinguished National Lab Fellow (2014 – present). She has thirty-four years of experience working in industry inventing and commercializing new technologies for major chemical manufacturing companies including Koch Industries, Lummus Technology, Dow, Dupont and ARCO Chemical Company. She has authored 155 publications and 257 patents. Dr. Gaffney is also a distinguished Joint Appointment Fellow at the University of South Carolina (2018 – present) where she is the Technical Director of the National Science Foundation Center for Rational Catalyst Synthesis. Some of her recent awards include: the 2019 American Chemical Society, Energy & Fuels, Distinguished Researcher Award in Petroleum Chemistry; the 2015 Eugene J. Houdry Award of the North American Catalysis Society; the Chemical Heritage Foundation, Women in Science Inductee, 2014; and the American Chemical Society, Industrial Chemistry Award, 2013. Dr. Gaffney received her BA in chemistry and mathematics from Mount Holyoke College and her Ph.D. in physical organic chemistry from University of Delaware.



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## DIRECTED C-H FUNCTIONALIZATION OF COMMON ORGANIC FRAMEWORK

**Haibo Ge**

*Texas Tech University, USA*

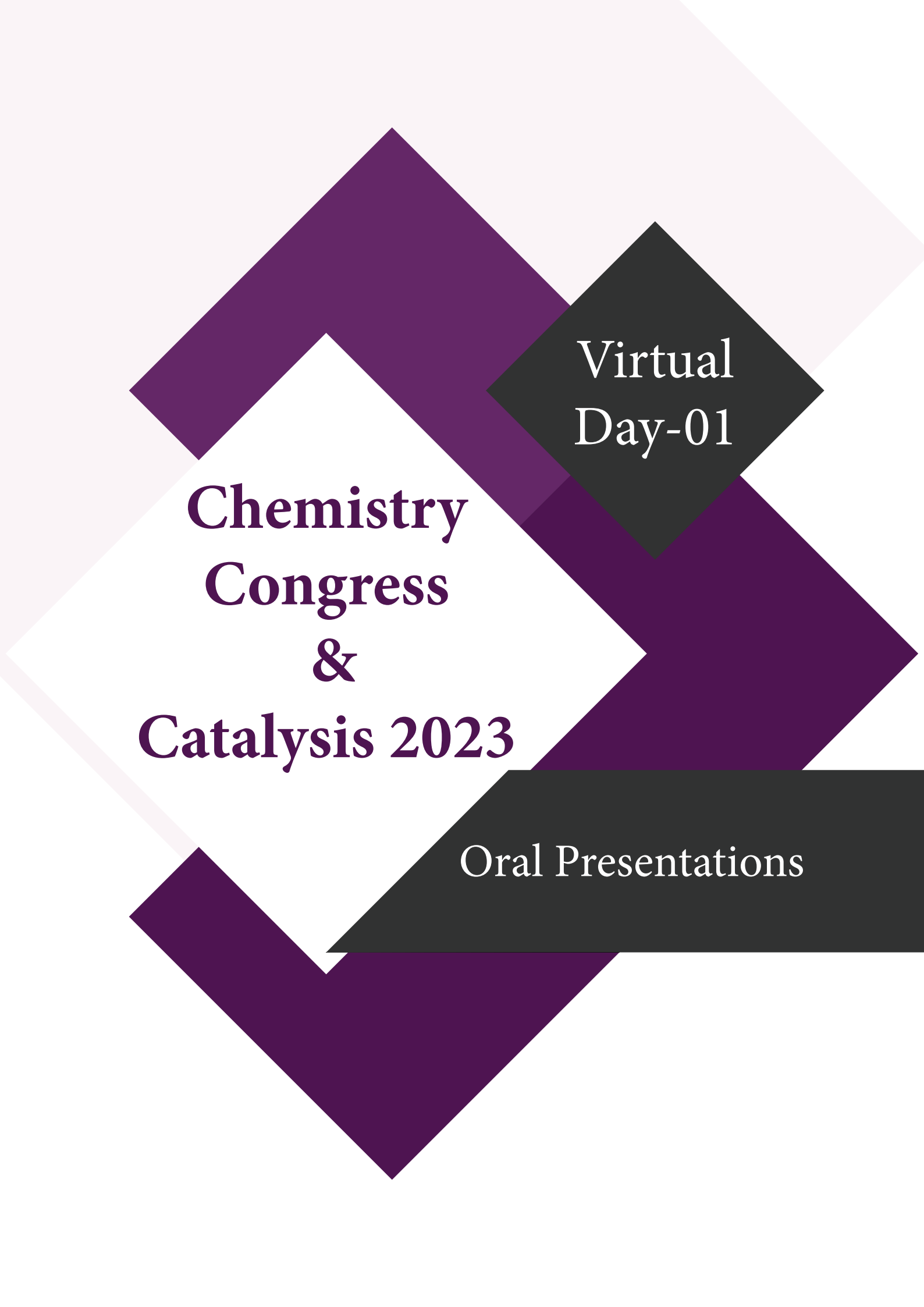
### Abstract:

Direct C–H bond functionalization represents one of the most efficient synthetic approaches in organic chemistry due to its atom and step economy and reduced waste generation. While aromatic C–H bond functionalization reactions have been extensively studied, this process with aliphatic substrates is challenging due to the high bond dissociation energy of a  $sp^3$  C–H bond and low polarity difference between the carbon and hydrogen atoms. 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 installation of a directing group and the subsequent removal after the desired operation severely hampers the efficacy and compatibility of the reactions. As such, the use of a common functional group such as amine, aldehyde, ketone, acid, etc, would be beneficial, and would advance the field of transition metal catalysis.

### 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. He had more than 60 publications including Nature Chemistry, Journal of the American Chemistry Society, Chem, Angewandte Chemie International Edition, etc





Virtual  
Day-01

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Oral Presentations

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## THE CATALYTIC ROLE OF ACETYLACETONATE COMPLEX COMPOUNDS OF VANADIUM(IV) IN THE POLYMERIZATION OF SELECTED OLEFINS

**Joanna Drzeżdżon**

*University of Gdansk, Poland*

### Abstract:

Plastics are present in every area of modern life. Over the last several decades, there has been a rapid development of research in the field of synthesis of new olefin polymerization catalysts. Contemporary research directions concern post-metallocene catalysts. A special group of catalysts for obtaining polyethylene and its copolymers, e.g. with 1-octene, are oxovanadium(IV) complex compounds. A new acetylacetonate (acac) complex of oxovanadium(IV) was synthesized and its catalytic properties in the polymerization of ethylene and copolymerization of ethylene with 1-octene were examined. The catalytic activities of the synthesized complex with acetylacetonate as a ligand and other acetylacetonate complexes such as  $V(acac)_3$  or  $VO(acac)_2$  were compared. All obtained products were examined multi-analytically using techniques such as size exclusion chromatography, differential scanning calorimetry, thermogravimetric method coupled with Fourier infrared spectroscopy. The results of catalytic studies on the newly synthesized oxovanadium(IV) acetylacetonate complex show that moderate insertion ratios equal to approximately 6% occur in the copolymerization products of ethylene and 1-octene.

### Biography

Joanna Drzeżdżon is an assistant professor at the Department of Environmental Technology, Faculty of Chemistry, University of Gdańsk. She obtained her PhD in 2017. Her scientific interests focus on olefin polymerization catalysts, including the application of "green chemistry" principles. She has published more than 50 academic papers in international journals, as well as 2 patents.

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## ENHANCEMENT OF THERMAL CONDUCTIVITY AND HEAT TRANSFER RATE INVOLVING HYBRID NANO FLUIDS ON MHD STAGNATION POINT FLOW OVER A STRETCHING SHEET

**Santoshi Misra**

*St. Ann's College for Women- Hyderabad, India*

### Abstract:

Nano fluids play a vital role in the world of industry and technology. With several market needs the research and advancement in Nano fluids and their applications has become significantly predominant. Nano fluids are Nano-metre sized particles suspended in base fluids like water, ethylene, glycol, oil etc., to enhance the thermal conductivity and heat transfer rate of energy transmission fluids in an economical way being cost effective. Hybrid Nano Fluids are a high end version having varied thermal applications and useful in industrial appliances working with high temperatures and are developed by diffusing two distinct forms of Nano particles in the base fluid. The research focuses on studying the behaviour of Hybrid Nano Fluid and its impact on the MHD Stagnation point flow over a stretching sheet. The highly non-linear governing equations of the fluid are transformed into ordinary differential equations using similarity transformations and reduced to first order for producing solvable equations. The 4<sup>th</sup> order RK method has been systematically employed for the further segregation to obtain accurate results equipped with shooting technique numerically. The effect of various dimensionless parameters like the Skin Friction, Nusselt number, Prandtl number, Eckert number, Lewis number, Biot number, Magnetic parameter, Thermophoresis parameter, Brownian motion on the Velocity, Temperature and Concentration profiles of the fluid flow are recoded and are in good agreement with the references used based on the results obtained from the graphs and tables in our research consistently showcasing the influences clearly.

### Biography

Santoshi Misra have over 19 years of teaching experience in mathematics for undergraduates and postgraduate students where in her career started as a computer science faculty teaching Microsoft Office and fundamentals of information technology for B.Com. students. Her interest and passion towards exploring different domains of work using my intellectual abilities to grow ahead has always been ceaseless. With a thoughtful mind and five years of her PhD research has left a remarkable growth in her level of understanding and perceiving knowledge where her wish to explore the world of learning and always ready to accept risk and challenges that come across and not just limit my profession to teaching. Currently working as Dean Student affairs and Assistant Professor-Department of Mathematics in St. Ann's College for women, Mehdiapatnam, Hyderabad, Telangana State.

## DEVELOPMENT OF OUTDOOR INCLINED PHOTOBIOREACTOR FOR ARTHROSPIRA PLATENSIS CULTURE: CONTROLLING SOLAR IRRADIANCE TO ENHANCE THE PRODUCTIVITY

**Tjandra Chrismadha, and Awalina Satya**

*National Research and Innovation Agency (of Republic Indonesia), Indonesia*

### Abstract:

Harmonizing natural solar radiation for optimal growth has been the major challenges in developing photobioreactors for outdoor microalgae and cyanobacterial cultures. This study aims to figure out all year long growth and productivity behaviour of *Arthrospira platensis* culture in respond to time dynamics solar light availability. A set of outdoor inclined plastic column photobioreactor for the cyacobacterial culture was installed on an open space roof, in line with recording of the daily natural solar irradiation every one minute, while 2 variation of plastic column sizes and 4 shading capacity paranets were appllied for the solar irradiance control. The culture assessment including parameters of culture density, specific growth rate, biomass productivity, chlorophyll and proximate content, as well as the phycocyanin productivity. From this six week experiment on semicontinuous mode, some correlation model of the assessed parameters and the average daily solar irradiance has been successfully established, revealed a possibility to manage risk of harmful peak open space daily solar irradiance, as well as improving the culture biomass and phycocyanin productivity both with the column size and paranet application. By prolonging the daily solar irradiance recording for a year long on 2022, this study demonstrated that the above established model can be useful for arranging a long time strategic measure in coping a particular local irradiance availability to enhance biomass or particular targeted products. Giving an example, this study showed that the estimated highest yearly volumetric productivity of  $63.20 \text{ g.L}^{-1}.\text{year}^{-1}$  can be achieved by combination of 13 cm diameter column and 70 % light shading paranet applications, while the same shading application in combination with wider 33 cm diameter column enhanced the highest culture areal productivity of  $6.08 \text{ kg.m}^{-2}.\text{year}^{-1}$ .

### Biography

Tjandra Chrismadha is a senior researcher in The National Research and Innovation Agency of Republic Indonesia. His expertise is to design culture system for improving aquatic plants bioproductivity. He has involved in photobioreactor development for algal and cyanobacterial cultures since the early 2000, and doing research for the scalling up and outdoor adaptation in the latest several years.



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## AN ADVANCED REVIEW ON THE CONTAMINATIONS OF WATER IN LEATHER AND FOOTWEAR MANUFACTURING INDUSTRY AND APPROPRIATE TREATMENT METHODS

**Suresh Aluvihara**

*University of Peradeniya, Sri Lanka*

### Abstract:

Leather and footwear manufacturing industry is a leading part of tannery industry which is an essential industry in the modern world. When considering the tannery processes and the nature of raw materials of leather, there can be found some sort of risks on the natural environment including the water contamination and pollution because of the generation of waste water and waste materials due to higher consumptions of a large number of chemical compounds including some toxic compounds in the process of tannery and the contents of the body parts of animals including biological matter and sewage matter. According to the current environmental norms, regulations and cleaner production technologies, the mitigation of environmental pollution would be an important factor in the reputation and the goodwill of the organization using eco-innovative methods and low cost methods. In the consideration of the major pollutants of the tannery industry which are released as tannery waste water, mostly there can be identified some excess amounts of acids, ions, dissolved solids, suspended solids, chlorides, sulfates, cadmium, lead, copper, mercury, arsenic, pesticides, organic pollutants, residues, oils and different types disease causing microorganisms (bacteria) in sewage wastes such as *Escherichia coli*, *Streptococcus lactis*, *Pseudomonas aeruginosa* and *Bacillus spp.* Therefore, it is possible to expect some severe impact on the quality of effluent water before the treatments and ultimately there will be affected some natural water bodies by the effluents unless having a proper treatment system and currently most of industries allocate a significant concern on different waste water treatment methods including some expensive methods and harmful methods. According to the outcomes and experiences of our researches and most of modern researches in water treatments, there were found some efficient results in the removal of most of above mentioned pollutants under the adsorption, absorption and filtration processes while using different earth materials and natural materials including clay, dolomite and burnt coconut shells in various physical forms. Eventually, it is possible to recommend those treatment methods to treat some tannery effluents to enhance the quality of effluent and the economy.

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## ENHANCED CATALYTIC ACTIVITY OF Pt/TiN NANOCOMPOSITES FOR CO OXIDATION AT LOW TEMPERATURES

**Evgeny Kabachkov**

*Russian Academy of Sciences, Russian Federation*

### Abstract:

The development of efficient and environmentally friendly catalysts for carbon monoxide (CO) oxidation at room temperature is of great importance for various industrial applications. Carbon monoxide is a toxic gas that poses a serious threat to human health and the environment. The development of efficient catalysts for CO oxidation is crucial to mitigate its harmful effects. In this study, we synthesized Pt/TiN catalysts and evaluated their catalytic activity towards CO oxidation at room temperature. Our results demonstrated that Pt/TiN catalysts exhibited excellent catalytic activity towards CO oxidation even at low temperatures. The high activity of these catalysts can be attributed to the synergistic effect between Pt and TiN, which enhances the adsorption and activation of CO molecules on the catalyst surface. We also investigated the effect of synthesis parameters on the catalytic performance of Pt/TiN catalysts. Our findings suggest that the particle size of Pt nanoparticles and the loading amount of Pt significantly affect the catalytic activity of Pt/TiN catalysts. Moreover, the addition of a reducing agent during the synthesis process can further improve the catalytic activity of Pt/TiN catalysts. The results of this study demonstrate that Pt/TiN nanocomposites have great potential as efficient catalysts for CO oxidation at room temperature. These catalysts can contribute to the development of sustainable industrial processes and environmental protection. The insights gained from this research can also guide the design and development of novel catalysts for future applications.

### Biography

Evgeny Kabachkov is a researcher in the field of chemical physics and medicinal chemistry. Research interests include catalysis, nanomaterials, XPS, CO oxidation, photocatalysis and environmental chemistry. The results of his work have been presented at numerous international conferences and published in more than 200 scientific articles in peer-reviewed journals. Currently, Evgeny Kabachkov works as a researcher at a leading federal research center, where he develops new catalysts for various applications

## WASTEWATER TREATMENT FOR REMOVAL OF TOXIC PHENOL USING BIOLOGICAL AND INDUSTRIAL WASTES AS ADSORBENTS

**Ashanendu Mandal**

*University of Calcutta, India*

### Abstract:

This research aims for adsorptive removal of phenol from wastewater by solid waste materials generated from biological wastes viz. guava tree bark, rice husk, neem leaves, activated carbon from coconut coir and industrial wastes viz. rice husk ash, red mud, clarified sludge from basic oxygen furnace, activated alumina. The adsorbents are characterized by SEM, XRD, FTIR and BET analyzers. The experiments of phenol removal are carried out with the variation of initial phenol concentration (5-500 mg/L), initial pH (2-12), adsorbent dose (0.10-20 gm/L), temperature (25-50°C) and contact time (30-600 min). The maximum phenol removal percentage through batch absorptions has been found to be as high as 97.50%. The kinetics analysis with the experimental results shows that the pseudo-second order model is best fitted for all adsorbents except red mud. The kinetic modelings show that the adsorption mechanism is supportive of film diffusion, intra-particle diffusion and chemisorption for all adsorbents. The isotherm analysis suggests that Freundlich isotherm model is best supportive for guava tree bark, rice husk, neem leaves, activated carbon, red mud and activated alumina, whereas Langmuir and D-R isotherm are best supportive for rice husk ash and clarified sludge respectively. The thermodynamics shows the spontaneity, randomness and endothermic/exothermic nature of the adsorption processes. The ANN modelling using two popular algorithms viz., Levenberg-Marquardt and Scaled Conjugate Gradient establishes that the experimental and predictive data are within allowable range. The scale-up designs are performed for their commercial applications. The regeneration and the safe disposal of used adsorbents are also studied for checking their wider industrial applicability. Further, the column study is also extensively carried out using the most efficient batch adsorbent neem leaves. The study concludes that these adsorbents can be used commercially for removal of toxic phenol from wastewater.

### Biography

Ashanendu Mandal has graduated as B. Sc in Chemistry and B. Tech in Chemical Engineering from University of Calcutta. He has got his M. Tech Degree in Chemical Engineering from IIT, Kharagpur. He has acquired MBA degree in Finance from IGNOU, New Delhi and has undertaken an Advanced Management Program from IIM Calcutta. He has also acquired the Degree of Ph. D. (Tech) in Chemical Engineering from University of Calcutta. Dr. Mandal has worked in ONGC for more than 34 years and his experience includes commissioning, modifications, safety, operations, artificial lifts, pressure maintenance, EOR and planning in offshore and onshore oilfields. He has also vast experience in marketing of upstream and downstream petroleum products. Dr. Mandal has published technical papers in Chemical Weekly and research papers in many international journals. He has visited more than 25 countries for attending training programs and for participating in international conferences as invited speaker or panelist. Dr. Mandal is a lifetime member of Indian Chemical Society and Indian Science Congress.

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## CATALYST FOR BIOFUEL PRODUCTION

**Muhammad Zubair**

*Quaid-I-Azam University, Pakistan*

### Abstract:

The prompt reduction of fossil fuel resources and their environmental effects has caused a serious threat to the humanity. Meanwhile, the exponential increase in the usage of fossil fuels by growth in world population, demands the exploration of new energy resources to overcome the energy crises. Biodiesel (mixture of alkyl monoesters) is indeed one of the appealing sources of energy. This research work mainly focused to develop new organic ligands and their complexation with organotin(IV) derivatives as catalysts for biodiesel production via transesterification. The synthesized ligands and their complexes have also been computationally studied to explore the structure properties relationship. We have preferred to synthesize various carboxylate ligands owing to their high donor/complexation capacity with organotin (IV). A series of carboxylate ligands (HL1 to HL10) have been synthesized via ring opening mechanism and were successfully characterized using various analytical techniques (FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, Single and crystal X-ray diffraction). From the experimental results, trigonal bipyramidal geometry and tetrahedral geometry were observed for triorganotin(IV) derivatives in both solution and solid state. In addition, trinuclear di-organotin(IV) complexes (C<sub>1</sub>-C<sub>4</sub>) were also synthesized and characterized with seven coordinated pentagonal bipyramidal geometry. The geometry, bond angle, and bond length were also studied computationally with density functional theory (DFT) and promisingly found highly aligned with the results obtained from the analytical techniques. All the synthesized complexes have been evaluated as homogeneous catalyst for the biodiesel production. The catalytic performance of the tested complexes was found as follow: triorganotin(IV) > diorganotin(IV) derivatives with maximum conversion efficiency of 92% and 64% respectively. The order of catalytic performance can be explained on the basis of steric and Lewis acidic character around the tin(IV) centre. However, trinuclear di-organotin(IV) complexes were found less active (26%) than tri/di-organotin(IV) that may be due to the high coordination number and therefore, Sn centre is less susceptible for nucleophilic attack. Moreover, the obtained castor oil biodiesel has been confirmed and quantified by FT-IR, NMR (<sup>1</sup>H and <sup>13</sup>C) and GC-MS. Keeping in view the catalytic performance of the screened compounds, it is expected that they might be the potential future candidates for the expansion of catalyst systems for efficient biodiesel production from the various precursors (vegetables oils).

## 4-CHLOROPHENOL ADSORPTION FROM WATER BY ACTIVATED CARBON FUNCTIONALIZED WITH AMINE GROUPS

**Mohammad Hadi Dehghani, Moslem Tazik, Kamyar Yaghmaeian, Shahrokh Nazmara, Mehdi Salari, Amir Hossein Mahvi, Simin Nasser, Hamed Soleimani, and Rama Rao Karri**

*Tehran University of Medical Sciences, Iran*

### Abstract:

4-Chlorophenol pollution is a significant environmental concern. In this study, powdered activated carbon modified with amine groups is synthesized and investigated its efficiency in removing 4-chlorophenols from aqueous environments. Response surface methodology (RSM) and central composite design (CCD) were used to investigate the effect of different parameters, including pH, contact time, adsorbent dosage, and initial 4-chlorophenol concentration, on 4-chlorophenol removal efficiency. The RSM-CCD approach was implemented in R software to design and analyze the experiments. The statistical analysis of variance (ANOVA) was used to describe the roles of effecting parameters on response. Isotherm and kinetic studies were done with three Langmuir, Freundlich, and Temkin isotherm models and four pseudo-first-order, pseudo-second-order, Elovich, and intraparticle kinetic models in both linear and non-linear forms. The synthesized adsorbent was characterized using X-ray diffraction (XRD), Fourier transforms infrared spectroscopy (FTIR), and scanning electron microscopy (SEM) analyses. The results showed that the synthesized modified activated carbon had a maximum adsorption capacity of 316.1 mg/g and exhibited high efficiency in removing 4-chlorophenols. The optimal conditions for the highest removal efficiency were an adsorbent dosage of 0.55 g/L, contact time of 35 min, initial concentration of 4-chlorophenol of 110 mg/L, and pH of 3. The thermodynamic study indicated that the adsorption process was exothermic and spontaneous. The synthesized adsorbent also showed excellent reusability even after five successive cycles. These findings demonstrate the potential of modified activated carbon as an effective method for removing 4-chlorophenols from aqueous environments and contributing to developing sustainable and efficient water treatment technologies.

## The STUDY OF THE CATALYTIC REFORMING PLANT AND THE PRODUCTION OF THE GASOLINE IN THE PETROLEUM REFINERY OF ARZEW-ALGERIA

**Menouar HANAFI**

*The University of Science and Technology of ORAN, Algeria*

### Abstract:

The catalytic reforming is a process of the petroleum refining , which is realized in specific conditions of the operations , and with chosen catalysts for the conversion of the naphtens and the paraffins to the aromatics and the isoparaffins.

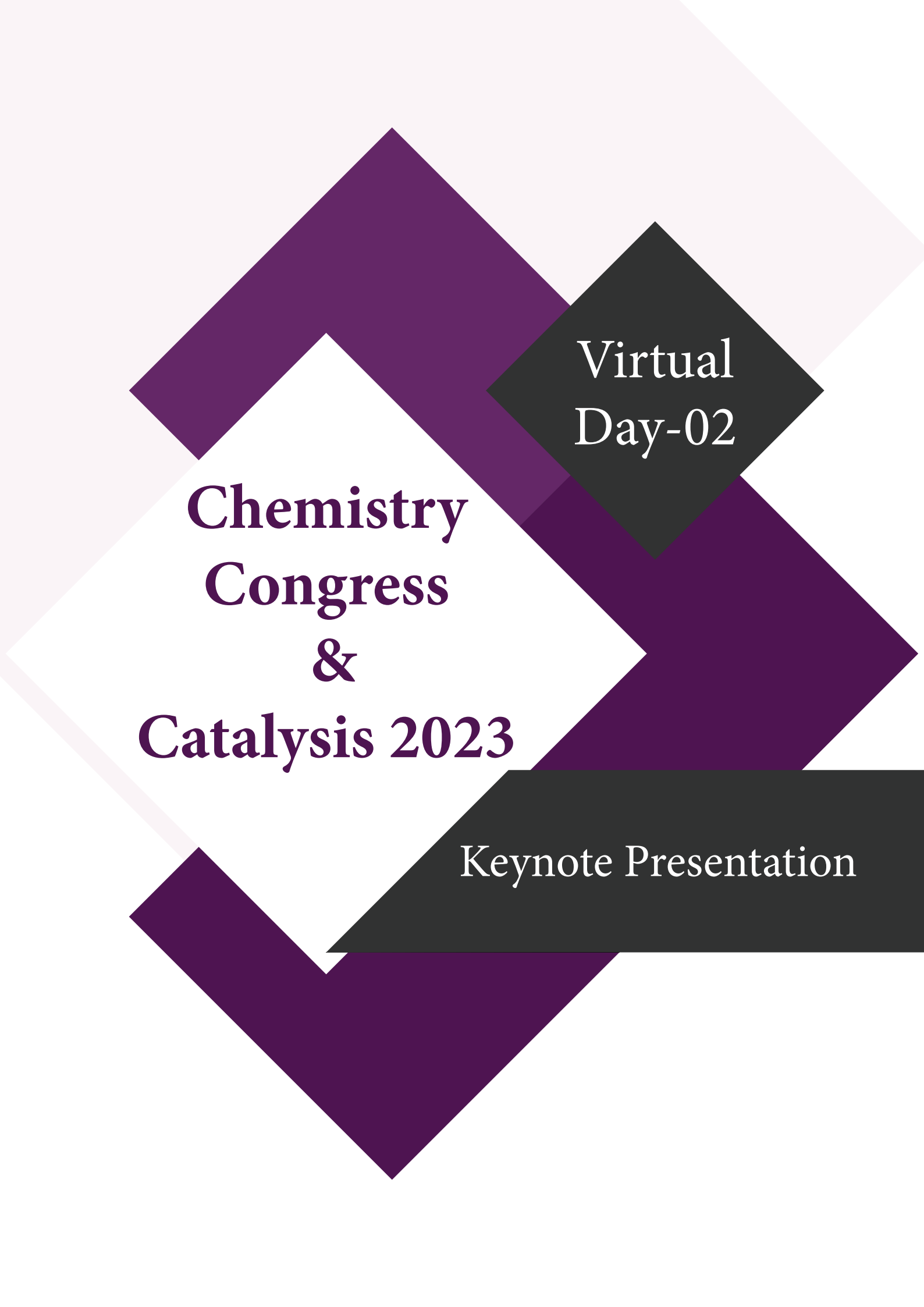
Two principal aims exist for this process :

- The production of the gasoline with a high octane number.
- The production of the aromatics hydrocarbons ( B . T . X . ) .

The quality of the catalyst , constitutes an important element of the realization of the catalytic reforming .For that , it is necessary the study of the principal following characteristics :

- 1) The activity.
- 2) The selectivity.
- 3) The stability.
- 4) The developments of the reforming catalysts:
  - a- The multifunctional catalyst.
  - b- The composition of the catalyst.
- 5) The poisoning of the catalysts of the catalytic reforming.
- 6) The disactivity of the catalysts.
- 7) The regeneration of the catalysts.





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Keynote Presentation

## SHAPE REVERSIBILITY AND CRYSTALLOGRAPHIC TRANSFORMATIONS IN SHAPE MEMORY ALLOYS

**Osman Adiguzel**

*Firat University, Turkey*

### Abstract:

A series of alloy materials take place in a class of advanced smart materials with the stimulus response to external effect. Shape memory alloys take place in this class by exhibiting a peculiar property called shape memory effect, with the chemical compositions in the beta phase field in phase diagrams. This phenomenon is characterized by the recoverability of two certain shapes of material in reversible way at different conditions. This phenomenon is initiated with thermomechanical processes on cooling and deformation and performed thermally in a temperature interval on heating and cooling, with which shape of materials cycles between original and deformed shapes in reversible way. Therefore, this behavior is called thermoelasticity.

Shape memory effect is result of the crystallographic transformations, thermally and stress induced martensitic transformations. Thermal induced martensitic transformation occurs on cooling with cooperative movements of atoms in  $\langle 110 \rangle$  -type directions on the  $\{110\}$  - type planes of austenite matrix, along with the lattice twinning reaction, and ordered parent phase structures turn into the twinned martensite structures. Twinned structures turn into the detwinned structures by means of stress induced martensitic transformation with deformation in the martensitic condition.

These alloys exhibit another property, called superelasticity, which is performed with stressing and releasing the material in elasticity limit at a constant temperature in parent phase region, and shape recovery is performed instantly and simultaneously upon releasing, by exhibiting elastic material behavior. Stress-strain profile is nonlinear in stress-strain diagram, also stressing and releasing paths are different, and hysteresis loops refers to energy dissipation. Superelasticity is also result of the stress induced martensitic transformation, and ordered parent phase structures turn into detwinned martensite structure with stressing. However, atomic bonds, grain boundaries, atom pair interactions, lattice vibrations (phonons) and other factors affect the transformations. Also, lattice twinning and detwinning reactions play important role in martensitic transformations. Copper based alloys exhibit this property in metastable  $\beta$ -phase region, which has bcc-based structures at the parent phase field. Lattice invariant shear and twinning is not uniform in these alloys and gives rise to the formation of complex layered structures. These structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences of atoms. In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on copper based CuAlMn and CuZnAl alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections. X-ray diffractograms taken in a long-time interval from the aged specimens at room temperature show that diffraction angles and peak intensities change with aging duration at room temperature. This result refers to the rearrangement of atoms in diffusive manner.

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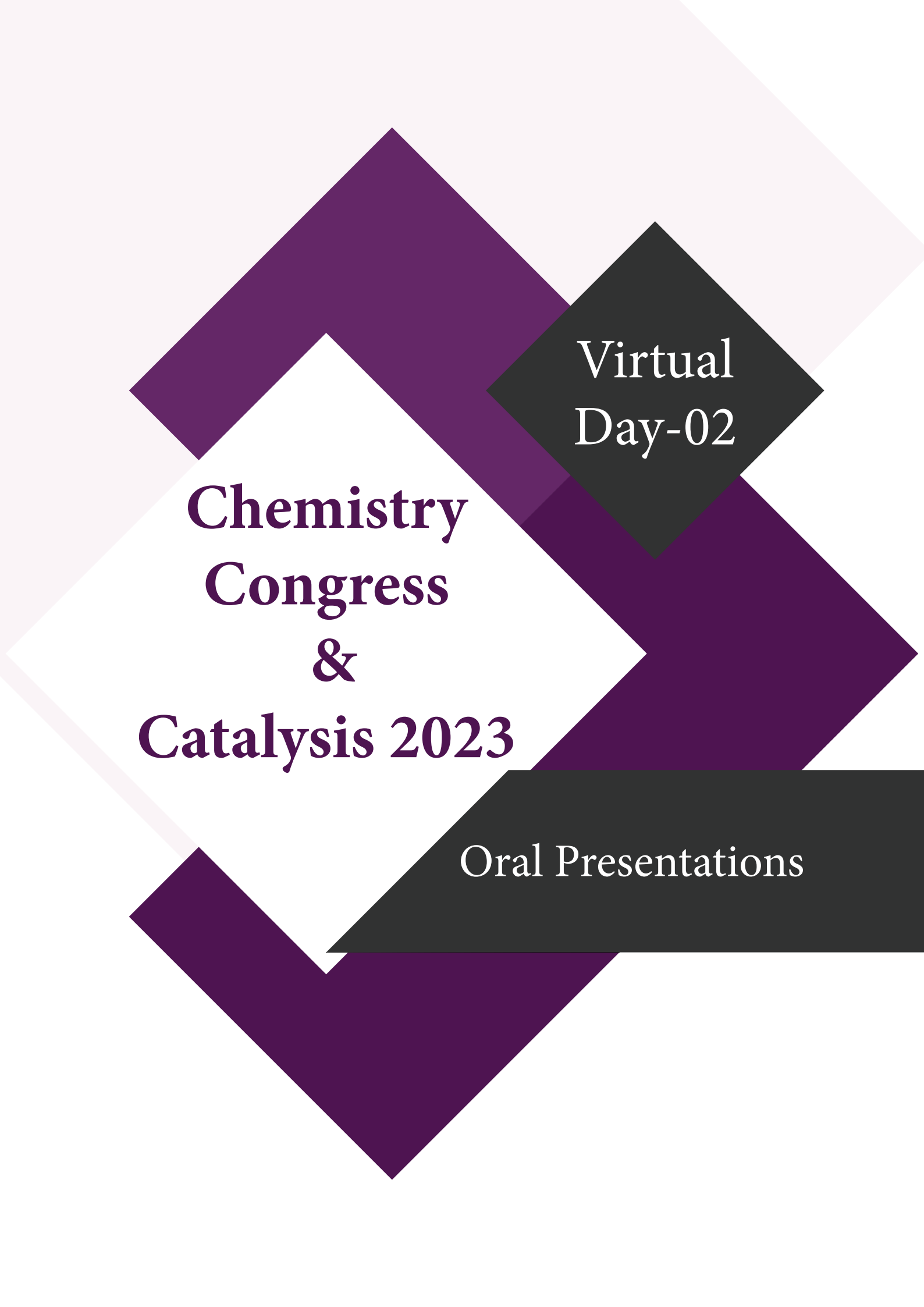


## Biography

Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post- doctoral research scientist in 1986-1987, and studied were focused on shape memory effect in shape memory alloys. His academic life started following graduation by attending an assistant to Dicle University in January 1975. He became professor in 1996 at Firat University in Turkey, and retired on November 28, 2019, due to the age limit of 67, following academic life of 45 years. He supervised 5 PhD- theses and 3 M. Sc- theses and published over 80 papers in international and national journals; He joined over 120 conferences and symposia in international level with contribution. He served the program chair or conference chair/co-chair in some of these activities. Also, he joined in last six years (2014 - 2019) over 60 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. Additionally, he joined over 120 online conferences in the same way in pandemic period of 2020-2022.

Dr. Adiguzel served his directorate of Graduate School of Natural and Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000. The ICDD (International Centre for Diffraction Data) also appreciates cooperation of his group and interest in Powder Diffraction File.





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## CHANGE OF THE FRACTIONAL COMPOSITION OF RESINS AND ASPHALTENES FROM HIGH VISCOSITY OIL IN THE PROCESS OF CATALYTIC AQUATHERMOLYSIS

Salih Indad Sh S, Irek I Mukhamatdinov and Alexey V Vahin

*Salahaddin University, Iraq*

### Abstract:

The resins and asphaltenes extracted from heavy oil sample of Ashalcha reservoir (Tatarstan, Russia) and the products of Co-based catalytic and non-catalytic aquathermolysis are investigated. Saturates and four subfractions of resins (C1-C4) different in color (C1-yellow, C2-orange, C3, C4-dark brown), are extracted by liquid adsorption chromatography method with individual and solvents also Five fractions of asphaltenes (A1-A5) the method stepwise extraction with an alcohol-benzene solvent with different alcohol content after precipitation of asphaltenes from oil with hot isooctane. In the process of catalytic aquathermolysis an increase in the content of light fractions is observed (saturated hydrocarbons) as a result of intensification of destructive hydrogenation, predominantly for the least durable –C–S–C– relations in molecules of resins and asphaltenes. Fractionation method leads to obtain more detail information about the structure of high molecular weight compounds due to subdividing large molecule and its aggregates into small ones. In the present studies, redistribution between resin and asphaltene fractions, extracted using solvents of various composition and dissolving strength, was found. The molecular weight of the resins is significantly increased from the first fraction of resins C1 to the C4 fraction. The molecular weight of each fraction of asphaltenes decreases as a result of the use of the catalyst.



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## ANALYSIS OF BLACK CARBON CONCENTRATIONS IN PM<sub>2.5-10</sub> AND PM<sub>2.5</sub> FRACTIONS BY MABI INSTRUMENT IN TWO URBAN AREAS OF DAKAR, SENEGAL

**Moustapha Kébé**

*University Cheikh Anta Diop Dakar, Senegal*

### Abstract:

Black carbon (BC) is a particular pollutant that absorbs visible light and can intervene in the climatic change with irradiance. The sources of BC emissions are known, such as incomplete combustion of fossil fuels and biomass burning. Our study focuses on two sites Hlm and Yoff in Dakar, Senegal in order to determine the mass absorption coefficient of BC in our polycarbonate nucleopore filters from November 2018 to October 2019 so as to collect PM<sub>2.5</sub> and PM<sub>2.5-10</sub> we face in our two study sites using MABI instrument. In addition, we investigate the source apportionment of black carbon in PM<sub>2.5</sub> fraction. We observe that the mass absorption coefficient of PM<sub>2.5</sub> is higher than that of PM<sub>2.5-10</sub>. The average concentration of BC at Hlm and Yoff were  $1.85 \pm 0.37$  and  $2.69 \pm 0.54 \mu\text{g.m}^{-3}$  respectively, whereas the average concentrations of BCBB were  $0.003 \pm 0.0007$  and  $0.08 \pm 0.01 \mu\text{g.m}^{-3}$ , respectively and for BCFF were  $1.85 \pm 0.37$  and  $2.61 \pm 0.53 \mu\text{g.m}^{-3}$ . The BC from at Yoff has two compounds with 2.97% of Biomass burning and 97, 03% of Fossil fuels in contrast to Hlm site the black carbon was mainly composed of fossil fuels in Dakar, the fossil fuels are mainly source of the black carbon.

### Biography

Moustapha Kébé completed his thesis in Atomic and Nuclear Physics at Cheikh Anta Diop University of Dakar. He is a part-time professor in the Department of Physics. I am author of some publications and currently the President of Optics Society America (OSA) in Senegal. His disciplines are Atmospheric Chemistry, Nuclear Chemistry and Environmental Chemistry.

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## CHIRAL PHOTOELECTRODES FOR EFFICIENT WATER SPLITTING

**Wilbert Mtangi, Rufaro Kawondera, Claudio Fontanesi, Marco Bonechi, Massimo Innocenti, and Gift Mehlana**

*Chinhoyi University of Technology, Zimbabwe*

### Abstract:

The ever increasing global climate challenges associated with greenhouse gas emissions call for the abandonment of fossil fuel sources in favour of alternative, sustainable green fuel sources. Hydrogen has been and will always remain as the ideal candidate to replace fossil fuel sources, owing to its higher energy density, absence of carbon and a benign combustion by-product. However, since the demonstration by Fujishima and Honda that hydrogen can be obtained by splitting water on a semiconductor surface by using light of a sufficient wavelength, the production of hydrogen through green and sustainable methods is still uneconomic and remains in the future. Despite the fact that the thermodynamic potential of producing the triplet oxygen molecule is lower than that of producing hydrogen peroxide, the formation of the peroxides is kinetically favourable since it occurs on a singlet surface and has no spin restriction constraints. Hence the water splitting process suffers high overpotential and the production of peroxides that compete with the production of the triplet oxygen molecule. In this paper, we demonstrate and present on the efficient production of hydrogen through photoelectrochemical water splitting by making use of chiral photoelectrodes in a photoelectrochemical cell. This is attributed to the efficient control of the electron spin, promoting the production of the triplet oxygen molecule, suppressing the production of peroxides and lowering the overpotential required for the photoelectrocatalytic water splitting process.

### Biography

Wilbert Mtangi is a renowned researcher in Materials Science and Engineering. He has a lot of expertise in the fabrication and characterization of electronic properties of semiconductor devices. He has published a lot of articles related to the characterization of defects in ZnO. He has a lot of passion in the development and characterization of photoelectrodes for generation of green hydrogen through photoelectrochemical water splitting and also the development of chiral perovskites for solar energy harvesting. This has seen him fabricate and characterize chiral photoelectrodes that have been used in improving the water splitting process based on the chirality induced spin selectivity effect. He is a recipient of the PhosAgro/IUPAC/UNESCO grant for Green chemistry and The World Academy of Science for Individual Scientists which have been targeted to pursue an innovative hydrogen generation project.

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## MASS TRANSFER COEFFICIENTS EVALUATION OF OXYTETRACYCLINE CATALYSIS: DIFFUSION THROUGH TiO<sub>2</sub>/SYNTHESIZED ACTIVATED CARBON COMPOSITES PROBLEM STATE

Djedouani Djamila and Chabani Malika

USTHB, Algeria

### Abstract:

Heterogeneous catalytic kinetics of organic compounds has been studied in several research works, but, the mechanism kinetics of these pollutants on the supported catalyst is rare and still poorly understood. In this research, we envisage to identify the appropriate kinetic mechanisms of the catalytic oxytetracycline degradation under UV- titanium dioxide- synthesized activated carbon systems. The reaction mechanism was investigated using single spherical pore-First-order reaction, and the effective diffusion coefficient 'D' was determined in order to measure how much the reaction rate is lowered because of the resistance to pore diffusion. The results show that the reaction is tremendously limited by the internal diffusion. There was a synergistic effect between synthesized activated carbon (CAPH) from peanut's hull and system UV+TiO<sub>2</sub> system. The mass transfer analysis in each phase alone of the composites (TiO<sub>2</sub> - CAPH) indicates that, the diffusion through the pore within the particle of CAPH pellet is 7.21 greater than diffusion throughout the TiO<sub>2</sub> catalyst pellet.

### Biography

Djedouani is a lecturer at the Houari Boumedienne University of Science and Technology in Algeria, a member of a research team at the reaction engineering laboratory of the faculty of process engineering.

## SYNTHESIS AND CATALYTIC APPLICATION OF MAGNETIC METAL FERRITE NANOPARTICLES IN ORGANIC REACTIONS

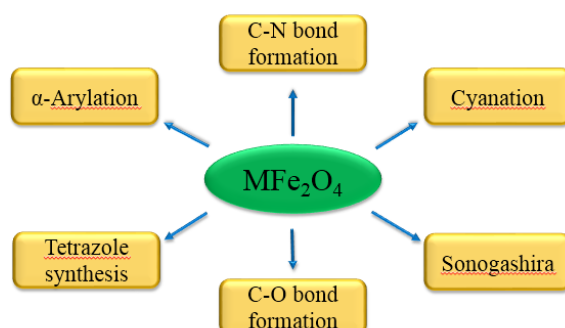
**Firouz Matloubi Moghaddam**

*Sharif University of Technology, Iran*

### Abstract:

Bimetallic nanoparticles are a class of nanomaterials with new physical and chemical properties resulting from synergistic effects between the two metals.  $MFe_2O_4$ , where M is a divalent transition metal, is the formula of one important family of these bimetallic compounds called metal ferrites. These structures crystallize in the spinel form showing superparamagnetic properties originating from the moment of antiparallel spines between ferric ions at tetrahedral sites and  $M^{2+}$  ions at octahedral sites. The unusual structural, electronic, magnetic and catalytic properties of these nanodimensional transition metal spinel oxides provide potential application in various fields, such as preparation of high density recording devices, gas sensors, and high efficient catalysts.

sFerrites used in catalytic applications are generally synthesized by low temperature co-precipitation methods which overcome the drawbacks such as low surface area, varying morphology, inhomogeneity at an atomistic level and large particle with grain boundary, generally associated with high temperature preparation. Further, co-precipitation methods generate Bronsted acid sites in different cationic environment in addition to Lewis sites, which makes the catalyst active and effective for many organic transformations such as aromatic alkylation, acylation, etc. It has been proved that these nanoparticles show very good catalytic activity in C-C and C-heteroatom bond formation. During the last couple of years, application of different types of these magnetic catalysts has shown in various organic transformations by our group. They have employed in C-N, C-O and C-C coupling reactions successfully; still, there are a lot more transformations that can be done using the catalytic properties of these compounds.



### Biography

Firouz Matloubi Moghaddam was born in Maragheh, Iran. He obtained his B.Sc. in Chemistry and M.Sc in Organic Chemistry from Tabriz University. Thereafter, he joined the group of Prof. G. Solladie in the University of Louis Pasteur Strasbourg France and obtained a 'Doctorat d'Etat' (Habilitation) in 1982. He also obtained a M.Sc in Medicinal Chemistry from the same University. After three years of postdoctoral appointments at University of Zurich (Prof.C.H.Eugster) and (Prof.A.Vasella), he began his own career at the Sharif University of Technology. Currently, he is distinguished professor of Organic Chemistry and his scientific interests include total synthesis of bioactive compounds, isolation, structure elucidation and synthesis of bioactive natural products, heterocyclic chemistry and catalysis

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## CEILING GRAPHENE: WIRELESS SYSTEM

**Amir Sepehri, Mohammad Kamal Ghassem Al-askari**

*Islamic Azad University, Iran*

### Abstract:

Over the last two decades, Graphene is classified as a promising material for new products in variety of industry. Based on laboratory experiment hetero-structure of graphene emerged unique properties in the domains of science and engineering. However, high prices and manufacturing in large quantities are still in the early stages. Expanding a new design solution is the essential requirement to overcoming challenges in the synthesis process. Herein, we are reporting a unique setup to accelerate production graphene. In this work the Magnetic energy systems used to unlimited charge energy running the system. Moreover, tesla coiled providing a wireless open system boundary to carrying electricity to activate Inspired the ceiling fan motion. In this way the graphite ingot is the core of the ceiling and graphite sheets play the role of ceiling fan blades. Laboratory analysis FE-SEM, FT-IR, UV-VISIBLE, XRD and Raman spectroscopy was down to characterizing the Nano particles. The result shows the ceiling fan design through a wireless open system provide large quantities of graphene with renewable energy resources completely free of charge. Ceiling graphene can open-up new opportunities for many industries to modify their products with the cheaper hetero- structure for Nanomaterials.

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