

9<sup>TH</sup> EDITION OF INTERNATIONAL CONFERENCE ON

# CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

October 21-22, 2021

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**CATALYSIS, CHEMICAL  
ENGINEERING AND TECHNOLOGY**

OCTOBER 21-22, 2021

**Theme:**

Exploring the advances and challenges in Catalysis and  
Chemical Engineering

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# *About* **MAGNUS GROUP**

**Magnus Group (MG)** is initiated to meet a need and to pursue collective goals of the scientific community specifically focusing in the field of Sciences, Engineering and technology to endorse exchanging of the ideas & knowledge which facilitate the collaboration between the scientists, academicians and researchers of same field or interdisciplinary research. Magnus group is proficient in organizing conferences, meetings, seminars and workshops with the ingenious and peerless speakers throughout the world providing you and your organization with broad range of networking opportunities to globalize your research and create your own identity. Our conference and workshops can be well titled as 'ocean of knowledge' where you can sail your boat and pick the pearls, leading the way for innovative research and strategies empowering the strength by overwhelming the complications associated with in the respective fields.

Participation from 90 different countries and 1090 different Universities have contributed to the success of our conferences. Our first International Conference was organized on Oncology and Radiology (ICOR) in Dubai, UAE. Our conferences usually run for 2-3 days completely covering Keynote & Oral sessions along with workshops and poster presentations. Our organization runs promptly with dedicated and proficient employees' managing different conferences throughout the world, without compromising service and quality.

## *About* **Catalysis 2021**

Magnus Group with gratification and privilege announcing its "9<sup>th</sup> Edition of International Conference on Catalysis, Chemical Engineering and Technology (Catalysis 2021)", an Online Event scheduled during October 21-22, 2021 with the theme "Exploring the advances and challenges in Catalysis and Chemical Engineering." The main aim of CATALYSIS 2021 is to provide interaction between Chemistry experts, Pharma industries, R&D department, Young Researchers, Ph.D. scholars, and other professionals in the areas of Catalysis and Chemical Engineering around the world to share about their research studies and new innovations in the field. You can increase your professional skills and discuss the practical challenges encountered and the solutions adopted.

KEYNOTE FORUM DAY  
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OCT 21-22, 2021

CATALYSIS 2021





**Teresa Poerio**

CNR-ITM, Irlay

## Catalytic and photocatalytic membrane reactors

The search for alternative methods to those applied for chemical production at an industrial level, such as reduction and oxidation processes, has become more intense. Many studies emphasize the innovative potentialities and the emerged role of the membrane reactors (MRs) for improving existing industrial processes and for introducing new production methodologies. With respect to conventional reactors, MRs can improve the efficiency of chemical conversion processes reducing reactants consumption and by-product formation (and also reducing polluting emissions) by controlling of the residence time of substrate molecules inside the reactor. The membrane allows not only the easy recovery and reuse of the catalyst, immobilized on the membrane or just maintained in suspension, but also the selective separation of the desired product from the reaction mixture contributing to limit side reactions. On this basis, improvements in terms of yield and selectivity can be expected. Higher energy efficiency, modularity, and easy scale-up are some other advantages of MRs with respect to conventional fixed bed reactors. In this work, particular attention is devoted to the reduction and oxidation production processes studied by our research group using various configurations of MRs and a photocatalytic membrane reactor.

### Audience Take Away:

- The audience will Improve the knowledge on the membrane reactor and they can use this approach in our lab.
- The audience can use this research to expand their research o for teaching purpose.
- This approach can solve the problems related to reactions limited by thermodynamic equilibrium

### Biography:

Dr. Teresa Poerio achieved her Master Degree in Chemistry (1999) at the University of Calabria under the supervision of prof. Giovanni De Munno, and she achieved the PhD (2006) in Chemical and Materials Engineering at University of Calabria under the supervision of prof. Raffaele Molinari. Since 2011, she is researcher at Institute on Membrane Technology. She is Advisor of several graduate students and co-supervisor of PhD students in collaboration with the University of Calabria. She is author of more than 70 publications in international journals, 10 books chapters and more than 100 contributions to national and international Congresses.



**Palanichamy Manikandan\*, Michael Balakos,  
Kazuhiko Shinyama**

Clariant Corporation

## Catalysts for Ethylbenzene to Styrene: Challenges & Breakthrough

Styrene is one of the major commodity chemicals/monomers used for the production of different polymeric materials such as polystyrene (PS), acrylonitrile-butadiene-styrene (ABS) and styrene-butadiene rubber, which find their use in several segments including packing materials, automotive, construction and tires. At present the world styrene production is over 35,000 kta, which is expected to reach over 50,000 kta in 10 years with a consumption growth rate of around 2% per annum. Styrene is predominantly produced by conventional dehydrogenation of ethylbenzene (EB) route in the presence of steam over Fe-based catalysts with different promoters using processes licensed by Badger or Lummus Technology. Being an endothermic process, selectivity to styrene and ethylbenzene conversion are controlled by heat, which is supplied through super-heated steam. In the conventional process, steam-to-hydrocarbon feed weight ratio (sometimes referred to as steam-to-oil ratio) is typically in the range of 1.0-2.0 with ethylbenzene conversion over 60% and styrene selectivity of more than 93%, where the by-products are mainly benzene and toluene due to the dealkylation reaction. Clariant Corporation is a styrene catalyst leader who offers a wide range of catalysts based on end use requirements. In this process, steam plays a crucial role such as in the removal of carbonaceous deposit (coke), as a diluent to shift equilibrium towards higher conversion. Steam, as an oxidizing agent, renders the iron oxide to remain in an appropriate oxidation state, and it supplies the needed heat for the reaction. However, the energy to produce the steam is expensive, resulting in a high operating expense. Therefore, Clariant endeavors to develop new-generation catalysts, which can be used at low steam-to-oil ratio of 1.0 or below. Loss or redistribution of promoter like potassium, building of carbonaceous deposits are major challenges while developing new commercial catalysts for low-steam operation. It is a real technical challenge to the catalysis community to develop a robust catalyst that works at this low steam-to-oil ratio, apart from other engineering challenges as it creates heat exchange limitations. Developing commercial scale catalyst production, which meets customer expectations, is a formidable scientific question. Some of the mechanistic aspects of the EB-to-styrene reaction and current challenges will be discussed along with our latest catalyst solutions.

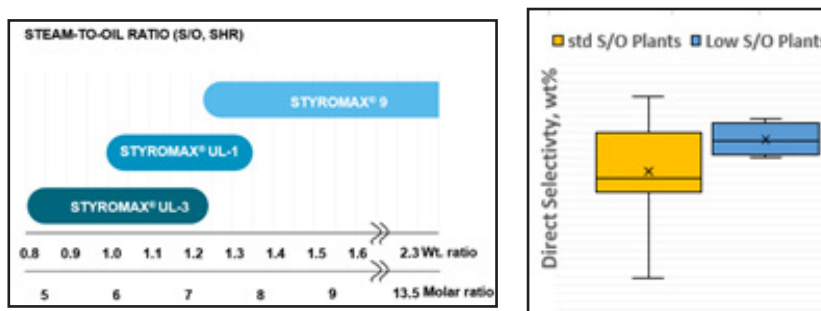
### Materials and Methods:

At present, Clariant offers the series of StyroMax® catalysts for standard steam-to-oil ratio and the StyroMax® UL series for (ultra-) low steam-to-oil ratio, which contain potassium promoted iron oxide along with other promoters. Typically, the catalysts are produced at lab scale/bench scale and tested before being produced at commercial scale. At every stage, the catalysts are tested for their performance against the reference catalysts. Their physical properties are measured before and after the reaction performance at certain process conditions.

### Results and Discussion:

Dehydrogenation of ethylbenzene involves multiple steps, starting from activation of ethylbenzene on the catalyst surface, abstraction of hydrogen from the activated EB with the subsequent formation of styrene. However, in this process, adsorbed styrene on the catalyst surface may tend to form carbonaceous materials (coke) if it is not desorbed quickly. Activated ethylbenzene can lean towards benzene if there is any acidity on the catalyst, or at high temperature. Kinetic and

thermodynamic factors play important roles. In order to maximize the EB conversion and styrene selectivity, one needs to add multiple promoters at an optimized loading, apart from suitable process conditions. The complexity becomes higher when steam-to-oil is reduced below 1.0 wt ratio. Clariant has been working on the continuous improvement of styrene catalysts (Figure 1, left) and offered different solutions to meet the requirements of either high conversion and high selectivity and/or a longer cycle length. It is gratifying to note that Clariant recently discovered a catalyst system with a formulation that yields higher average selectivity even at low steam-to-oil ratio, which is a real breakthrough (Figure 1, right).



**Figure 1.** Left: Different catalysts developed for ethylbenzene dehydrogenation to styrene reaction that can be operated in a range of steam-to-oil (S/O) ratios. Right: Styrene selectivity performance comparison of standard S/O ratio and low S/O ratio operations.

## Significance

Achieving a high conversion rate of ethylbenzene along with a high selectivity to styrene, especially at low steam-to-oil ratio, is important as it saves cost and energy, which also improves the overall sustainability. With a continuous improvement effort, Clariant has developed a robust catalyst, which works well at a low S/O ratio and also shows improved overall performance.

## Audience Take Away:

How important to develop high performance catalysts to saves cost and energy, which also improves the overall sustainability

Why it is essential to understand the fundamental reaction pathways while designing a high-performance catalyst

Developing a catalyst which finds use at commercial scale does not happen overnight and it is critical to pay attention to many aspects including catalyst composition, treatment/process conditions, experimental data, customer feedback etc. while improving the catalyst performance.

## Biography:

Dr Manikandan received his Ph.D. in Chemistry from Indian Institute of Technology Madras in 1998. After three years of post-doc at Weizmann Institute of Science and Northwestern University, he joined National Chemical Laboratory, India as a Catalysis Scientist in 2001. He moved to Dow Chemicals R&D in 2007 where he was leading the catalysis team before joining SABIC R&D in Bangalore where he a Senior Manager for glycols. Currently, he is a senior group leader with Clariant, Louisville, USA. He has 40 publications, 6 US patents and helped the companies to save millions of dollars through improved process and catalysts.





**Dr. Deepak Ganta**

Texas A&M International University, USA

## Nanomaterial as catalysts in photoelectrochemical energy conversion and hydrophobic recovery

Natural plant-based dye-sensitized solar cells (DSSCs) gained significance due to their low cost, non-toxicity, environmental friendliness and availability. Plant dyes serve as a sensitizer, which absorbs sunlight and converts solar energy into electric energy with the aid of titanium oxide nanomaterials who serve as catalysts. The motivation for this work is to explore natural pigments from non-toxic plants, which can survive in dry conditions, and abundant in nature, with simple and inexpensive extraction methods. Further, upon extraction investigate methods for fabricating DSSCs from the combination of natural plant-based dye extracts. Two types of natural plant-based dyes extracted from Cladode and a leaf of Aloe Vera are used. The working electrode was fabricated from Titanium dioxide ( $\text{TiO}_2$ ) nanopowder, which provides a wide band-gap and serves as an electron transporter and carbon coated Fluorine-doped Tin Oxide (FTO) conductive glass served as the counter electrode. When light is incident on the plant-based dye, the electrons from the dye are absorbed by Titanium dioxide nanomaterial and further leading to the charge separation via the electrolyte. Optical properties of the dye were investigated with UV-Vis Absorption Spectroscopy. Fourier Transform Infrared Spectroscopy (FTIR) technique was used to study the surface chemistry of the plant dyes before the fabrication of DSSCs. In conclusion, the DSSC sensitized by the Cladode offered the highest conversion efficiency of 0.740%, amongst the other DSSCs, due to the presence of stronger adhesion promoters in the chlorophyll dye, providing a better charge transfer. We overcame the problems in mixing the dyes by designing a DSSC using two dyes on a side-by-side configuration, reporting a conversion efficiency of 0.50%. Overall, natural plant-based dyes as sensitizers of DSSCs were promising because of their low-production costs, simple and energy-efficient assembly methods, and environmental friendliness. We will also discuss current work on the wearable solar cells. Additionally, the ability to modify the contact angle of water on silicon has applications ranging from thermal management of electronics to miniaturized biomedical and microfluidic devices. The motivation for this part of the work is to explore simpler oxygen plasma treatments that can both expand the overall range of contact angles and ensure long-term behavior. Through simple variation in the thickness and oxygen plasma treatment, we were able to integrate both hydrophobic and superhydrophobic surface on the same sample. The variation in contact angle arises from choosing nanowires of different lengths as catalysts. Nanowires are grown by metal assisted chemical etching and are (1-3) D in shape. We characterize the surfaces using a combination of X-ray photoelectron spectroscopy (XPS), contact angle measurements, and ellipsometry. Taken together with contact angles available from similar treatment on bulk silicon, it is possible to lithographically create regions of diverse contact angles, from  $\sim 5^\circ$  to  $\sim 149^\circ$ .

### Audience Take Away:

- They will learn how to fabricate solar cells and learn function of nanomaterials in energy conversion
- They will gain exposure to various analysis methods to test materials
- They will learn to fabricate Silicon Nanowires (1-3) D on a chip
- They will learn how to develop nanostructures based coating solutions or products
- They will learn about photovoltaics and green energy

## **Biography:**

Dr. Deepak Ganta received his M.S in Electrical Engineering and Ph.D. in Electrical Engineering and Physics from Oklahoma State University. He is currently an Associate professor in Engineering at TAMIU. Before joining TAMIU, Dr. Ganta worked as a senior scientist at ngimat and as a post-doc at UIUC. His interdisciplinary research is in the area of micro/nanotechnology, flexible optoelectronics, soft robotics, e-textiles, energy conversion, and advanced materials analysis. He has published over 50 articles in peer-reviewed journals and conference proceedings, including 24+ journal papers in journals including Materials Research Express, IEEE J. Sel. Topics Quantum Electronics, Surface Science Spectra, Measurement Science and Technology, AIP Advances, Chemical Physics Letters, and J. Chem. Physics. He has contributed to three book chapters in Advances in Solar Energy Research. Energy, Environment, and Sustainability (Springer) and Advances in Nanotechnology. He secured grants from NSF, DoD and Texas Higher Education Coordinating Board. His research work earned both national and international media coverage. His biography was listed in Who's Who in America 2014 edition and he received the key scientific article honor from advances in engineering.



**Yuyuan Zhao**

University of Liverpool, United Kingdom

## Hierarchical porous metals manufactured by powder metallurgy and De-alloying

This presentation gives a short overview of the characteristic properties of porous metals manufactured by powder metallurgy based space-holder methods. In this family of methods, a metal powder is first mixed with a filler material in the powder form. The mixture is then compacted and subsequently sintered to form a metal network. The filler material is removed either before, or during, or after the sintering to generate the pores in the resultant porous metal. The as-produced porous metals have distinctive porous structures. In effect, the pores are negative replicas of the particles of the filler material and the porosity is determined by the volume fraction of the filler material in the powder mixture preform. Pore shape, pore size and porosity can all be controlled accurately. The functionality of the porous metals derives from the combinations of distinctive characteristics of the solid and gaseous phases. The solid phase provides geometrical architecture, strength, electrical conductivity, thermal conductivity, magnetic shielding, acoustic barrier etc., while the gaseous phase offers compressibility and allows fluids to flow through. This presentation focuses on recent developments in the manufacture of hierarchical porous structures composed of micro- and nano-scale pores by combining a space-holder method and a de-alloying process.

### Audience Take Away:

- An overview of manufacturing technologies for porous metals
- A novel process combining powder metallurgy and de-alloying for producing hierarchical structures.
- Techniques for measuring surface areas and fluid permeability.

### Biography:

Professor Zhao obtained his BEng and MSc degrees from Dalian University of Technology and a DPhil from Oxford University. He worked as a Lecturer at Dalian University of Technology and a Research Fellow at Birmingham University before he joined Liverpool University in 1998. His current research interests are in the manufacture, characterisation and application of porous materials. He was awarded the prestigious Ivor Jenkins Medal in 2015 by the Institute of Materials, Minerals and Mining for an outstanding contribution to powder metallurgy

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SPEAKERS

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**Keyur D. Bhatt**

Ganpat University, India

## Highly efficient functionalized calix[4]pyrrole wrapped scrupulous nano-palladium catalyst

**C**alix(4)pyrrole-palladium nanoparticles synthesis with the help of meso-modified hydroxy calix(4)pyrrole (OHCP) derivatives. OHCP-PdNPs utilized for the C-C coupling reactions as an efficient nanocatalyst. This study includes the stability as well as pH studies of fine PdNPs. OHCP is an electron-rich ligand that is capable of reducing as well as encapsulate the metal ions because of the availability of electron-rich hydrazide functional group and H-bonding promoter four pyrrole units. In comparison with normal hydrazine, CP-hydrazide has a higher withdrawal ability, so Pd-NPs periphery is surrounded by them and undergoes stronger web-like capping on palladium. Similarly, OHCP-PdNPs are aqueous and air stable, besides affordable alternatives for the synthesis of stable PdNPs. Moreover, encapsulating the periphery of PdNPs using OHCP enhances its activity and selectivity. This recognition may lead to numerous promising applications towards an efficient catalytic activity.

### Audience Take Away:

- How to synthesize metal nanoparticles from supramolecules.
- How metal nanoparticle used for the catalytic reactions.
- Catalytic performance of metal nanoparticle upon coupling reactions

### Biography:

Dr. Keyur D. Bhatt received his bachelors in Chemistry and Masters of Science in Pharmaceutical/Organic Chemistry from the Sardar Patel University, Vidhyanagar, Gujarat, India in 2008 after which he worked Chemist at Asian Paints Ltd. & ICAR for one year till 2009. After that he joined Ph. D (2009-13) from Department of Chemistry Gujarat University, Ahmedabad Gujarat under UGC-BSR Scholarship. He served more than 12 year in teaching and research in Department of Chemistry, School of Sciences, Gujarat University, Chemistry Department, C. U. Shah University, and currently working as an Associate Professor & Head, Department of Chemistry, Ganpat University from June 2017 till now. He visited London UK for international faculty development program. He delivered invited lectures in many national and international conferences. He has successfully guided 78 students through their Master. Dissertation, 7 M. Phil and 3 Ph. D students. He has 02 Indian patents, 62 Research articles and 16 books in International Journals to his credit. Area of interest and specialization: To Design Synthesis, Characterization of Supramolecule, Fluorescence sensors and Nanoparticles.



**Goncagul Emir, Direncan Engindeniz, Ozgur Arar\***

Ege University, Turkey

## **Sustainable removal of Phosphate from aqueous solutions by Electrodeionization (EDI)**

Phosphorus is widely used in agriculture and industry. It is an important substance in the human body but excessive phosphorus in the water system may cause environmental problems known as eutrophication. In this work, the electrodeionization (EDI) technique was applied for the removal of phosphate from aqueous solutions. The effect of applied potential, the flow rate of phosphate-containing solution, the concentration of electrolyte circulated in electrode compartments, pH of the solution as well as interfering ions on the removal of phosphate were investigated. Solution pH has a notable effect on the removal rate. At pH 2, 83% of phosphate was removed from the solution while it was 97% at pH 6 and 12. When the applied potential was increased from 10V to 15V removal rate increased from 93% to 97%. The presence of interfering ions did not affect the removal rate.

### **Audience Take Away:**

- Principles of Electrodeionization system.
- Effect of process parameters on phosphate removal.
- Electroregeneration of ion-exchange resins

### **Biography:**

Dr. Arar studied Chemistry at the Ege University, Turkey and graduated as MS in 2004. He received his PhD degree in 2012 at the same university. Dr. Özgür Arar (M), is well-experienced research chemist who specialises in the field of water treatment. His work currently focuses on membrane processes including, electrodialysis (ED), electrodeionization (EDI) and pressuredriven membrane processes such as reverse osmosis (RO) and ultrafiltration (UF). Moreover, Dr. Arar has experience in sorption processes and has considerable research output on water treatment by ion exchange resins. Furthermore, Dr. Arar works on preparation and modification of polymers and biopolymers for water treatment. He has published more than 30 research articles in SCI(E) journals.

**Orlando Elguera**

Universidade de São Paulo, Brazil

## **Review of research topics for scaling-up of Sonochemical reactors (Sono-reactors)**

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

### **Biography:**

Orlando Elguera is currently working as Doctor of Science with Major in Analytical and Inorganic Chemistry, Universidade de São Paulo, São Paulo Brasil.



**Hyeyoung Shin**

Chungnam National University, Republic of Korea

## Computational design of highly active electrocatalysts for oxygen evolution reaction

Electrocatalyst is a key component to applications of electrochemistry in energy and environment. Metal oxides/oxyhydroxides are promising electrocatalysts beyond metals which have been mainly used as electrocatalysts but suffered from its intrinsic limitation in the optimization of performance. However, atomistic understanding of electrochemical reactions on metal oxides/oxyhydroxides have not been studied extensively because some metal oxides/oxyhydroxides feature localized unpaired spins and thus demand theory beyond the standard density functional approximations. Here, we apply a state-of-the-art theoretical method, using the hybrid functional and explicit constant electrochemical potential calculations to unravel the atomistic mechanism underlying the optimal performance of nickel oxyhydroxide based catalysts for oxygen evolution reaction (OER). This predicts dramatic improvement in performance of the nickel oxyhydroxide based catalysts for OER and also suggests a strategy to accurately describe the electrochemical processes as a function of explicit chemical potential.

### Audience Take Away:

- A strategy to accurately describe the electrochemical processes based on computational chemistry.
- A guideline to design highly active nickel oxyhydroxide based electrocatalysts for OER

### Biography:

Dr. Shin is an assistant professor at the Graduate School of Energy Science and Technology (GEST), Chungnam National University, Korea. She received her PhD in theoretical chemistry from Korea Advanced Institute of Science and Technology (KAIST) in 2016. Her main research interests focus on developing new materials and its application to renewable energy systems.





**V. Dappe, Karima. Ben Tayeb Karima\*, H. Vezin, S. Mariette, O. Serve, V. Livadaris**

University of Lille, France

## Characterization of petroleum fractions by in situ EPR spectroscopy

The behavior and the structural properties of organic radical species (ORs) in their native hydrocarbon environment as a function of temperature was investigated by electron paramagnetic resonance spectroscopy (EPR). Five petroleum fractions derived from the same initial crude oil were studied in the temperature range of 293-673K. Results from continuous wave (CW) and pulsed EPR spectroscopy show petroleum fractions behave differently under thermal activation. The inverse of the normalized area versus the temperature gave us different slopes changes in accordance with the generation and the recombination of ORs. The EPR experimental parameters (lineshape, linewidth) highlighted that during the thermal treatment, no conformational change occurred but impact the organic matter maturity with the breaking of sulfur chains.

### Audience Take Away:

- The aim of this contribution is to assess the possibilities of the EPR spectroscopy to provide information on the behavior of petroleum fractions.
- The scientist community will be interested by this presentation which highlighted the benefice of EPR technique that is almost never used in the oil world.
- The understanding of the structure and the behavior of compounds present in petroleum fractions could improve the conversion of the heavier crude oil fractions. Indeed, the conversion of heavy crude oils causes numerous problems due to their inherently poor qualities.

### Biography:

Dr. Ben Tayeb studied Chemistry at the Lille University, France and graduated as MS in 2006. She then joined the research group of Prof. Fournier and Lamonier at the catalysis unit and solid-state chemistry (UCCS) in France. She received her PhD degree in 2009 at the same institution. After two-year postdoctoral fellowship supervised by Dr Pinard at the Institute of Chemistry (IC2MP) in France, she obtained the position of an Associate Professor at the LASIR, in Lille University.



**Antonia Iazzetti\*, Antonella Goggiamani, and Giancarlo Fabrizi**

Catholic University of Sacred Heart, Italy

## Palladium-catalyzed benzylic-like nucleophilic substitution of benzofuran-2-ylmethyl acetate with N, S, O and C soft nucleophiles

The benzo[b]furan core is a motif present in several natural and unnatural pharmacologically active compounds exhibiting various biological properties including anti-inflammatory, anti-oxidant, anti-arrhythmic, hemostatic, antimicrobial, anti-viral, antifungal, and anti-tumor activities and are antagonists for the H3 receptor and angiotensin II.<sup>1</sup> Particularly, 1-(benzofuran-2-ylmethyl)-4-benzylpiperazine (Figure 1) has been selected as lead compound for  $\alpha_1$  receptor affinity and selectivity over the  $\alpha_2$  receptor.<sup>2</sup>

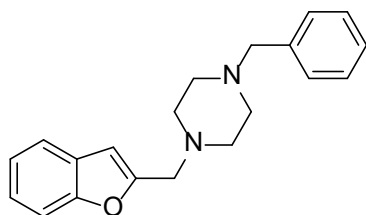
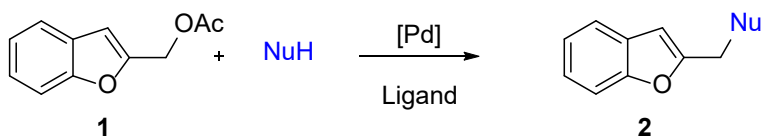


Figure 1. 1-(benzofuran-2-ylmethyl)-4-benzylpiperazine

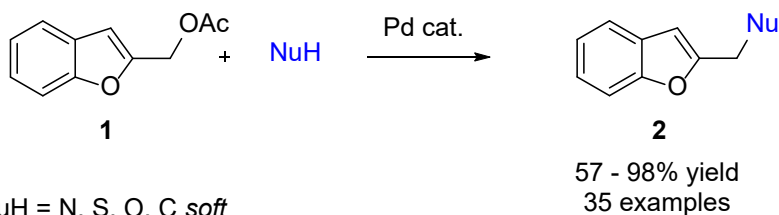
Due to the remarkable properties of compounds this compound, we decided to develop a new protocol for the preparation of variously substituted 2-(aminomethyl)benzo [b]furans evaluating the possibility that benzofuran-2-ylmethyl acetate **1** could undergo a palladium-catalyzed benzylic-like nucleophilic substitution in the presence of various nucleophiles (Scheme 1) to afford the 2-(aminomethyl)benzo[b]furan structure **2**.



NuH = N, S, O, C *soft*

### Scheme 1: Work Hypothesis

Results of our investigation, summarized in the scheme 2, showed that the catalytic system dramatically influence the reaction outcome: with nitrogen based nucleophiles the reaction works well with  $\text{Pd}_2(\text{dba})_3/\text{dppf}$ , while with sulfur, oxygen and carbo-nucleophiles  $[\text{Pd}(\eta^3\text{-C}_3\text{H}_5)\text{Cl}]_2/\text{XPhos}$  is more efficient. Furthermore, the reaction revealed to be regioselective since the nucleophilic substitution occurs only on the benzylic position of the  $\eta^3$ -(benzofuryl)methyl complex.



NuH = N, S, O, C *soft*

Ps Cat:  $\text{Pd}_2\text{dba}_3/\text{dppf}$  or  $[\text{Pd}(\eta^3\text{-C}_3\text{H}_5)\text{Cl}]_2/\text{XPhos}$

**Scheme 2:** Palladium-catalyzed benzylic-like nucleophilic substitution of benzofuran-2-ylmethyl acetate with N, S, O and C *soft* nucleophiles.<sup>3</sup>

The usually high to excellent yields and the simplicity of the experimental procedure make this method particularly convenient for the preparation of this class of compounds.

The main detail of our investigation will be discussed during the presentation.

#### Audience Take Away:

- The proposed methodology could be of interest for the chemists involved in the study of palladium catalyzed reactions, in the synthesis and/or functionalization of benzofuran derivatives, and in the development of new drugs.
- The method allows to easily obtain a class of compounds of interest in various field of chemistry including medicinal chemistry, organic synthesis, and organometallic chemistry. The high yields and the simplicity of handling make this procedure very advantageous and useful for their preparation.

#### Biography:

Antonia Iazzetti is professor assistant at Catholic University of the Sacred Heart of Rome. Since her PhD in Pharmaceutical Science at Sapienza University of Rome in 2013, she worked in the field of organometallic chemistry focusing on the transition metal-mediated synthesis of heterocycles. Recently, working in the frame of a relevant European research project (Horizon 2020), she has aimed to the valorization of industrial by-products developing innovative and sustainable extraction/purification/concentration technology to be applied to the recovery of valuable compound from production side-streams. She is author of more than 30 scientific publications in international journals indexed by Scopus and WOS.



**Mayra E. Manzanera-Estrada\*, Marisela Cruz-Ramírez, Marcos Flores-Alamo, José Miguel Gracia y Jiménez, Rodrigo Galindo-Murillo, Juan Carlos García-Ramos, Lena Ruiz-Azuara, Luis Ortiz-Frade**

Instituto Tecnológico Superior Zacatecas Sur, Av. Tecnológico No. 100, Col. Las Moritas, Tlaltenango, Zacatecas, México; mayra.me@zacatecassur.tecnm.mx.

### **Effect of tunable redox behavior of bis chelate substituted 1, 10-phenanthroline Cu(II) complexes on its reaction with superoxide anion in DMSO. Toward a simple criterion to identify a SOD-like mechanism**

In this work we report a series of Cu(II) complexes  $[\text{Cu}(\text{N-N})_2(\text{X})]^+$ , ( $\text{N-N}$  = substituted 1,10-phenanthroline derivatives and  $\text{X} = \text{Cl}^-$  or  $\text{NO}_3^-$ ), with tunable  $E_{1/2}$  for electrochemical reduction  $[\text{CuII}(\text{N-N})_2(\text{X})]^+ + 1e^- \rightarrow [\text{CuI}(\text{N-N})_2] + \text{X}^-$ . The disproportionation of  $\text{O}_2^{\bullet-}$  was explored in presence of the electro-generated species  $[\text{CuI}(\text{N-N})_2]$  using cyclic voltammetry in a non-aqueous media, arising a new simple method to propose a SOD-like mechanism, which can be used as a quick guide test for a compound, before being proven in biological assays. It was found that complexes with high negative half wave potential values ( $E_{1/2}$ ) for Cu(II)/Cu(I) couple shown a current increment for oxygen reduction, related to the capability of the disproportionation of this reactive oxygen species.

#### **Biography:**

Dra. Mayra studied Chemical engineering at the Universidad Autónoma de Zacatecas, México and graduated as Ms in Electrochemical in 2012. She then joined the research group of Prof. Ortiz-Frade at the Centro de Investigación y Desarrollo Tecnológico en Electroquímica. She received her PhD degree in 2016 at the same institution. She has published 5 research.



**Nguyen Anh Duc, Bence Balterer, Gyorgyi Szarka, Attila Domjan, Bela Iván and Ervin Kovacs\***

Research Centre for Natural Sciences, Hungary

## Green solvents as a new tool for olefin metathesis

Olefin metathesis plays an important role in the field of pharmaceuticals, materials and petrochemical processes. Olefin metathesis is a catalytic process which involves a pair of carbon-carbon double bonds to be rearranged in order to form new products. This can be more valuable compared to the starting ones. Generally for this reaction halogenated solvents (chloroform, dichloromethane), aromatics (benzene, toluene), THF are used. Due to the success of olefin metathesis in large scale industries, more greener solvents are desired to decrease the environmental impacts of this transformation process. In this work, we have studied the effect of green solvents compared to dichloromethane on ring-opening metathesis polymerisation (ROMP), ring-closing metathesis (RCM) and isomerization reactions with three commonly used ruthenium based Grubbs type catalysts in olefin metathesis.

To compare the conditions and catalysts, kinetic measurements have been carried out for all the reactions using <sup>1</sup>H NMR. Besides, the polymers obtained by ROMP were characterized by gel permeation chromatography (GPC).

The green solvents were proved to be very effective tool in the reactions carried out in our model experiments.

### Audience Take Away:

- Using green chemistry can be an easy solution to avoid toxic and hazardous solvents in different types of olefin metathesis reactions.
- The purity of the solvent and the oxygen free conditions have key role in olefin metathesis reactions.
- These circumstances can be feasible economically in industrial scales also.

### Biography:

Dr. Ervin Kovács studied chemical engineering at the Budapest University of Technology and Economics, Hungary where he received his MSc and his PhD degree (2015). After three years postdoctoral fellowship at the Metathesis Research Group at Research Center of Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary he joined to the group of Prof. Michael Greaney at School of Chemistry, University of Manchester, UK as a postdoctoral research associate. Dr. Ervin Kovács obtained the position of Research Associate in 2019 in Polymer Chemistry Research Group, Research Center of Natural Sciences, Hungary.



**Ashanendu Mandal**

Doctorate In Chemical Engineering At University Of Calcutta, India

## Adsorptive removal of toxic phenol from industrial wastewater using low-cost adsorbents

Phenol being toxic in nature needs to be removed from wastewater before its discharge. This research aims for removal of phenol through adsorption process using several low-cost adsorbents. Four bio-adsorbents such as guava tree bark, rice husk, neem leaves, activated carbon from coconut coir and four industrial waste adsorbents such as rice husk ash, red mud, clarified sludge from basic oxygen furnace, activated alumina were used in this research work. The surface characterization of the adsorbents were carried out by SEM, XRD, FTIR and BET analyzers. The phenol removal percentage by the adsorbents were investigated through batch experiments 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 removal percentage was obtained as high as 97.50%. The experimental results were used for kinetic study which showed that the pseudo-second order was best fitted for all adsorbents except red mud and the adsorption mechanism was supportive of film diffusion, intra-particle diffusion and chemisorption for all adsorbents. The isotherm analysis suggested that Freundlich isotherm model was best supportive for guava tree bark, rice husk, neem leaves, activated carbon, red mud and activated alumina, whereas Langmuir and D-R isotherm was best supportive for rice husk ash and clarified sludge respectively. The thermodynamics study successfully revealed the spontaneity, randomness and endothermic / exothermic nature of the adsorption process for each adsorbent. The adsorption experiments were also performed with the real industrial wastewater collected from a coke oven plant. The innovative ANN modelling using two popular algorithms viz., Levenberg-Marquardt and Scaled Conjugate Gradient was studied which established that the experimental and predictive data were within the allowable range. The scale-up designs and the safe disposal of used adsorbents were studied for examination of their commercial applications. The regeneration of the adsorbents were studied using distilled water and ethanol solution separately to find out their regeneration efficiency. The research finally reveals that all the adsorbents are effective for phenol removal to a large extent and thus can generate substantial circular economy.

### Biography:

Ashanendu Mandal done his M.Tech in Chemical Engineering, Indian Institute of Technology, Kharagpur ,MBA in Finance, Indira Gandhi National Open University, New Delhi and Pursuing Doctorate in Chemical Engineering at University of Calcutta, India. he is being trained in Petroleum Production Engineering, Indian School of Mines, Dhanbad Offshore Maintenance, IHRDC, Houston, USA and Calgary, Canada, Contract management, Indian Institute of Management (IIM), Calcutta, Personal Survival and Survival Craft, LBS Nautical and Engineering College, Mumbai, Environmental Clearance Procedure for Oil & Gas, Institute of Petroleum Safety, Health & Environment Management, Goa, Pipeline Corrosion, NACE International, India section, Mumbai, Well Productivity Model, Institute of Oil & Gas Production Technology, Mumbai, Advanced Environmental Management Systems Auditing, Det Norske Veritas (DNV), India section, Stimulation Technology & Specialized Production Services, Institute of Management Development, Dehradun, Petroleum Pacific International, Conference Connections, Singapore, BPR, Benchmarking & ERP Implementation, Xavier Institute of Management, Bhubaneswar, Advanced Management Programme, Indian Institute of Management (IIM), Calcutta

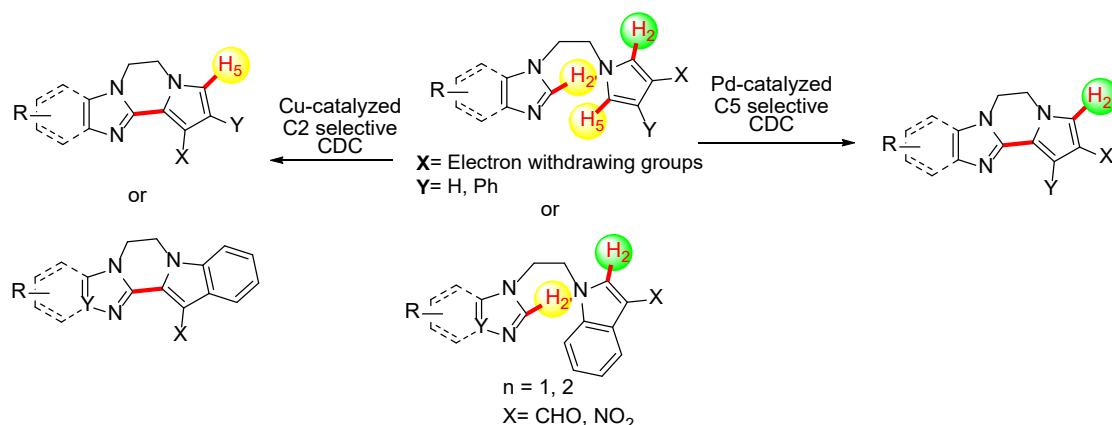


**Devalina Ray**

Amity University, India

## Transition Metal-Catalyzed Site-Selective C-H Functionalization of N-Heteroaromatics

Nitrogen containing heterocycles and their analogues are ubiquitous organic scaffolds found in nature and are known as medicinally important pharmacophores, among which azoles, pyrroles, indoles and quinolines have the most frequent occurrence. Hence, the synthetic exploration and expansion of their applications is critical for realizing their full potential. The inherent reactivity of these heteroarenes has enabled direct bond formation even in unfunctionalized scaffolds through transition-metal catalysis. In this context, the Cu-catalyzed site selective C<sub>2</sub>-H activation followed by intramolecular cross dehydrogenative coupling (CDC) of 3-substituted pyrroles and indole derivatives was established for direct access to polycyclic heteroarenes in moderate to good yields. Interestingly, the Pd-catalyzed reaction conditions for 3-substituted pyrrole derivatives preferred C<sub>5</sub>-selective intramolecular CDC over C<sub>2</sub>-selective products (Scheme 1). Further, as an advancement towards regioselective C-H functionalization of N-heteroaromatics, transition-metal free intermolecular C<sub>5</sub>-H chalcogenation of 8-aminoquinolines was developed under mild reaction conditions. The successful implementation of this methodology was further established through late-stage derivatization of pamaquine analogue which is known to be an efficient antimalarial.



Scheme 1: Transition metal-catalyzed C2 and C5-selective CDC of N-heteroaromatics



**Haider Almkhelfe\*, Placidus B. Amama**

Kansas State University, Iraq

## **Supercritical fluids as reaction media for scalable production of carbon nanomaterials**

**W**e have demonstrated scalable and selective synthesis of carbon nanotubes (CNTs), carbon nanofibers (CNFs), and onion-like carbon (OLC) in a batch reactor using supercritical fluids (SCF) as reaction media. The process utilizes toluene and alcohols (ethanol, propanol, and butanol) as carbon precursors in combination with ferrocene. Growth with supercritical toluene at 600°C in the absence of water yield large-diameter CNTs and CNFs while the introduction of 2.78 mmol/L of water enhances the product yield by 50% and promotes the formation of smaller-diameter CNTs and the exterior surface of CNTs was decorated with Fe nanoparticles. At 400°C, in the absence of water, supercritical toluene produces mainly OLCs and the selectivity increases with introduction of water, peaking at 5.55 mol/L. For alcohols, there is a gradual evolution of the morphology of nanocarbons formed from mainly OLCs as the ratio of C/O atoms increases to tube like structures, possibly due to a decrease in the tendency of graphitic sheets to minimize their energies by curling into onion-like structures as chain length increases. This study provides a framework for utilizing SCF reaction media in a batch reactor to achieve scalable and selective growth of different nanocarbons and nanocarbon-metal nanocomposites.





**Rocio Redon**

National Autonomous University of Mexico, Mexico

## Heck catalysis of palladium nanoparticles obtained in different reducing systems

Palladium(0) nanoparticles have been widely used in cross coupling reactions, including Heck reactions. For this study, we obtained palladium(0) nanoparticles in colloidal suspension using different combinations of solvents and reducing methods under aerobic conditions. The variation in systems used to synthesize palladium(0) nanoparticles resulted in different nanoparticle sizes. To investigate whether the particle size had an effect on catalysis, we used two different temperature and reaction times as reaction conditions, without the use of stabilizing agents, other than the solvent and/or the anions in the initial nanoparticle synthesis. All of the palladium nanoparticles investigated, worked in the cross coupling C-C Heck reaction, but yields did not show appreciable differences when high temperature and long reaction times promote a high reduction of palladium(II). With the use of lower temperature and reaction time, the differences start to be observed. The best C-C catalysis conversion was observed when N,N-dimethylformamide was used as solvent in the absence of reducing agent and with sodium citrate as reducing agent. The obtained size of the nanoparticles act as a reservoir of soluble palladium species that behave as the true catalyst.

### Audience Take Away:

- This study reports the influence of stabilizers, temperature, solvents and reducing agents on the formation of Pd nanoparticles and their efficacy in the Heck cross-coupling reaction between bromobenzene and styrene. Working on aerobic conditions, thus the reaction costs can be reduced.
- It is a complete account on the above-mentioned parameters and how they affect the catalytic conversion of the two substrates.
- The “cocktail” based catalysis is now well-accepted as a way to explain some of the catalytic phenomena, and in most cases smaller NPs leaching from larger conglomerates is nowadays a well-established rationalization.
- The current research addresses some of the pertinent parameters that may influence this leaching, and comparative results (in particular those obtained at lower reaction temperature, 120 °C) show that additive-free Pd NP catalysis is feasible.

### Biography:

Dr. Rocío Redón obtained her B. Sc. in Chemistry in 1993 at the Universidad Nacional Autónoma de México and her Ph. D. in the same University, in 2002. During her Ph. D. studies, she had the opportunity of joined different Chemistry research groups, in 1997 and 1998 with Prof J.R. Dilworth at Essex and Oxford Universities; in 1998 with Prof. Ana Albeniz, and with Prof. Craig Jensen from 1998 to 2001 at Hawaii University. She also joined the research group of Ashok Kakkar in McGill University from 2012 to 2013. Finally, after one year of postdoctoral fellowship she obtained the position of an Associate Professor at the Universidad Nacional Autónoma de México, where she actually works on the synthesis and characterization dendrimers and nanocomposites dendrimer-noble metal NPs, studying their potential catalytic applications and drug delivery properties. She has published more than 40 research articles in SCI(E) journals.



**Riam Abu Much**

The Academic Arab College for Education in Haifa, Israel

## Teaching and learning Chemistry in context with Nanotechnology applications

Nanoscience and nanotechnology (NST) are at the forefront of modern science in the 21st century. Nanotechnology applications are penetrating all aspects of society, affecting humans' everyday life and needs, in addition to their great contribution to the prosperity of the world-wide economy. Therefore, future teachers, students, and undergraduates need to achieve certain knowledge in nanoscience in order to navigate the science-based issues related to their everyday lives and societal aspects and to intelligently question and understand the ethical and societal implications of these revolutionary technologies. Teaching in "context" is characterized by the use of social, technical or scientific contexts as a starting point for developing an understanding of chemistry and creation chemistry more relevant to students' daily lives. Nanoscience and its applications are good candidates for teaching in the "context" of science education because they have clear connections to students' daily lives, have industrial aspects and all represent a rich environment involving research, society, and industry. The present study focuses on developing nanotechnology education program that connect between basic concepts in science with aspects in nanoscience and its applications.

### Audience Take Away:

- The presentation contributes to nanoscience and nanotechnology education and underlying its basic aspects
- It provides an idea for developing laboratory experiments as an effective method for teaching nanoscience and nanotechnology
- Providing the skills of transforming a complex scientific experiment into a simple one with educational objectives

### Biography:

Dr. Riam is currently the Head of the Chemistry Department at The Academic Arab College of Education in Haifa, Israel, and a Senior Lecturer at the same college. She earned her Ph.D. degree in Chemistry (Nanoscience and Nanotechnology) from Bar-Ilan University, she also received her M.Sc. and BSc. In Chemistry from the Hebrew University of Jerusalem. In 2008-2009 she was a post-doctoral fellow in Chemistry on Bar-Ilan University and served as teaching assistant at Bar-Ilan University. Recently, she started to deal with Nano Education. Among the awards she has received is the "Best Paper Award" for the best paper presented at any of the ICSEETS 2017.



**H. Boucheloukh\*, S. Rouissa, N. Aoun, M. Beloucifa, T. Sehili, F. Parrino, V. Loddo**

University of Constantine, Algeria

## **Degradation of non-steroidal drug under solar irradiation In the presence of Nickelate nanopowders**

To optimize water purification and wastewater treatment by heterogeneous photocatalysis we utilize a  $\text{NiFe}_2\text{O}_4$  or as a catalyst and solar irradiation as a source of energy. In this concept an organic substance present in many industrial effluents was chosen: naproxen ((S)-6-methoxy- $\alpha$ -methyl-2-naphthaleneacetic acid or 2-(6-methoxynaphthalenyl) propanoic) a non-steroidal anti-inflammatory drug. The main objective of this study is to degrade naproxen by an iron and nickel catalyst, the degradation of this organic pollutant by nickel ferrite has been studied in a heterogeneous aqueous medium, with the study of the various factors influencing the photo catalyzes thus: the material concentration and the acidity of the medium. The photocatalytic activity was followed by HPLC-UV and UV-Vis spectroscopy. A first order kinetic model appropriately fitted the experimental data. The degradation of naproxen was also studied in the presence of  $\text{H}_2\text{O}_2$  as well as in an aqueous solution. The new hetero-system  $\text{NiFe}_2\text{O}_4$ /oxalic acid is also discussed. The fastest naproxen degradation was obtained with  $\text{NiFe}_2\text{O}_4/\text{H}_2\text{O}_2$ . In a first-place, we detailed the characteristics of the material  $\text{NiFe}_2\text{O}_4$  which was synthesized by the sol-gel methods, using various analytical techniques: visible UV spectrophotometry, X-ray diffraction, FTIR, cyclic voltammetry, luminescent discharge optical emission spectroscopy.

**Keywords:** Naproxen, Nickelate, photocatalysis, Irradiation



**F.V. Yusubov, M.F. Mirbabayev\***

Azerbaijan Technical University, Azerbaijan

## Mathematical modeling of the adsorption process with variable conditions

The proposed work is devoted to the study of the adsorption process of  $H_2S/N_2/CO_2$  gas mixtures with variable pressure. The basis for calculating the process of adsorption separation of gas mixtures is a mathematical model of heat and mass transfer processes, which consists of the following equations:

Differential equation in partial derivatives of the material balance of the adsorbed substance

$$\frac{\partial C_i(r, \tau)}{\partial \tau} = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 k(C_i) \frac{\partial C_i(r, \tau)}{\partial r} \right] \quad i = 1, N \quad (1)$$

Differential equation in partial derivatives of the heat balance of the adsorbed substance

$$\frac{\partial T}{\partial \tau} = \frac{\lambda}{C_a} \cdot \frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) + \alpha_a (T - \theta) + q \frac{\partial C_i}{\partial \tau} \quad (2)$$

$$\text{Kinetic laws of the adsorption process} \quad \frac{1}{D_i} \cdot \frac{\partial a_i}{\partial \tau} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial a_i}{\partial r} \right) \quad (3)$$

Differential equation of pressure change according to the Mendeleeev-Chaperon equation

$$\frac{\partial P}{\partial \tau} - \frac{P}{T} \frac{\partial T}{\partial \tau} = R_1 T \frac{\partial C_i}{\partial \tau} \quad (4)$$

Equilibria in the form of the Langmuir equation:

$$a_i = \frac{a_m \cdot b_1 \cdot P_i}{1 + \sum_{i=1}^n b_1 \cdot P_i} \quad (5)$$

where  $C_i$  is the concentration of the adsorptive,  $a_i$  is the concentration of the adsorbate,  $P$  is the pressure,  $r$  is the current radius of the adsorbent grain,  $\tau$  is the adsorption time,  $k$  is the constant,  $T$  is the adsorption temperature,  $\theta$  is the local temperature,  $R$  is the universal gas constant,  $q$  is the heat adsorption,  $\alpha$  is the volumetric heat transfer coefficient;  $\lambda$  is the heat transfer coefficient (adsorbent grains),  $C_a$  is the heat capacity per unit volume of the adsorbent,  $D_i$  is the diffusion coefficient,  $a_m$  is the limiting amount of adsorbate,  $b_1$  is a constant. In addition, the equilibrium non-isothermal process of adsorption in a grain

of a spherical adsorbent is expressed by the equation  $a=f(c,r)$ . At the same time, the concept of the average concentration of adsorbent, adsorbate and temperature is used:

$$\begin{aligned}\overline{C}_i(\tau) &= \frac{3}{R} \int_0^R c \cdot r^2 dr, & \overline{a}_i(\tau) &= \frac{3}{R} \int_0^R a r^2 dr \\ \overline{T}(\tau) &= \frac{3}{R} \int_0^R T r^2 dr\end{aligned}\quad (6)$$

where  $R$  is the radius of the adsorbent grain;  $r$  is the current radius of the adsorbent grain;  $\tau$ -time if we take:

$$L = R \left( \frac{a-b}{3\beta} + \frac{R}{15 D_i} \right), \quad \frac{V_a}{V} = n$$

where  $V_a$  is the volume of the adsorbent,  $V$  is the volume of the adsorbent bed of the adsorber,  $L$  is the height of the adsorbent bed,  $a_0$  is the initial concentration of the adsorbate,  $m$  and  $b$  are constants. As a result of several mathematical operations, equations (1-5) are obtained:

$$\begin{aligned}C_i(\tau) &= \frac{n \left( \frac{a-b}{m} - a_0 \right)}{1+n(a-b)} \cdot e^{-\frac{1+n \left( \frac{a-b}{m} \right)}{L} \cdot \tau} + \frac{C_0 + n \cdot a_0}{1 + \left( \frac{a-b}{m} \right) \cdot n}, & \psi &= \frac{a-b}{m} \\ C_i(\tau) &= \frac{n \cdot (\psi - a_0)}{1+n \cdot (a-b)} \cdot e^{-\frac{1+n \cdot \psi}{L} \cdot \tau} + \frac{C_0 + n \cdot a_0}{1 + \psi \cdot n}\end{aligned}\quad (7)$$

Using the above model, consisting of equations (1-5) and solutions (7), we calculated the adsorptive concentration along the fixed bed of the adsorbent, showing that the adsorptive concentrations obtained at the outlet are controlled by the pressure drop in the fixed bed of zeolite in the adsorber, depending on from the flow rate of the incoming gas.

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**Pierre. M. Chevalier<sup>1\*</sup>, Zhanjie Li, Zhenbin Niu**

R&D Department, Dow Silicones Belgium SPRL, Seneffe, Belgium

R&D Department, Dow Silicones Corporation, Auburn, MI, USA

## **$\beta$ -Alkynol inhibition in Ru/Pt dual catalysis for hydrosilylation of silicones**

The platinum-catalyzed hydrosilylation reaction between a silicon-hydrogen and a carbon-carbon double bond is one of the foundational chemistries for the silicone industry. Since first reported in 1957, this addition reaction has been extensively used for the industrial production of intermediates and to form three-dimensional crosslinked networks into a wide range of cured performance silicones such as into fluids, coatings, sealants, rubbers and composites for building and construction, personal care, and pressure sensitive adhesives markets to name a few.  $\beta$ -Alkynol inhibitors play a determinant role in this Karstedt-catalyzed hydrosilylation providing a long working time or bath life at room temperature, while allowing for rapid command cure at elevated temperature, being paramount for viable industrial processes. Using <sup>13</sup>C-labeled 1-ethynyl-1-cyclohexanol (<sup>13</sup>C-1)  $\beta$ -alkynol inhibitor in a SiH/SiVinyl reactive model system, it was possible to monitor the composition change by Nuclear Magnetic Resonance spectroscopy during cure showing that <sup>13</sup>C-1 was selectively consumed by Pt-catalysed hydrosilylation with the Si-H group despite the large excess of reactive vinyl siloxanes. This hydrosilylation selectivity of terminal alkyne over vinyl and the temperature dependent kinetics are keys to the inhibition mechanism. We wish to report here the Ru/Pt dual catalysis to lower the cure temperature while maintaining a suitable working time through the evaluation of a range of Ru-complexes leading to the identification of [Cp\*Ru(MeCN)<sub>3</sub>]<sup>+</sup>OTf<sup>-</sup> complex promoting the selective ruthenium-catalyzed alkyne hydrosilylation of the inhibitor thus triggering the platinum-catalyzed olefin hydrosilylation and crosslinking at a cure temperature as low as 85OC and within 4 seconds, being critical for industrial silicone release coating applications onto low heat deflection temperature (HDT) commodity plastic substrates.

### **Audience Take Away:**

- It covers catalyzed addition reactions and selectivity between olefins and alkyne which is applied much beyond organosilicon chemistry. Yet it will open-up people to silicon chemistry as a sound alternative to fossil-based organic materials
- Industrial needs, processes, and limitations will be discussed in terms of bath life, crosslinking chemistries, cure kinetic control. Specific Ru and Pt complexes will be reviewed with conversion rate, time, and temperature, parameters surely also investigated within the audience's research
- The design of experiments coupled with the use of labelled element and the translation into a real industrial case such as siliconized liner for the labelling market shall help the audience in determining the path in their current research methodology down to industrial application

### **Biography:**

Dr. Chevalier received his Ph.D. in Organometallic Chemistry from the University of Montpellier in 1995 under the supervision of Pr. R.J.P Corriu from the French Science Academy. He spent 25 years in various research and managerial roles at Dow Corning and more recently Dow Chemical research centers in Great-Britain and Belgium. Dr. Chevalier is currently a Principal Scientist within the European Resins, Coating and Adhesives Product Development team at Dow Silicones Belgium responsible in developing and commercializing new innovative technologies in the Pressure Sensitive Industry. He holds 32 patents and has published 23 research articles, and 4 book chapters.



## Bunsho Ohtani\* and Mai Takashima

Institute for Catalysis, Hokkaido University, Sapporo 2R&D Department, Dow  
Silicones Corporation, Auburn, MI, USA

### True design and characterization of catalyst and photocatalyst materials through electron trap-distribution analyses

How can we design solid photocatalysts? What is the decisive factor controlling photocatalytic activities? So-called band-structure model (BSM), electrons in a valence band (VB) of a photocatalyst is photoexcited to a conduction band (CB), leaving positive holes in VB, and electrons and holes reduce and oxidize, respectively, substrates adsorbed on the surface of the photocatalyst, does suggest preferable band positions for redox reaction uniquely decided only by crystalline structure. The other possible factors, e.g., particle size and surface structure, cannot be discussed within BSM. Recently, we have developed reversed double-beam photoacoustic spectroscopy (RDB-PAS) which enables measure energy-resolved density of electron traps (ERDT). Those electron traps (ETs) seem to be predominantly located on the surface of almost all the metal oxide particles, with exception of nickel oxide and therefore they reflect macroscopic surface structure in ERDT patterns. Using ERDT pattern with the data of CB-bottom position (CBB), i.e., ERDT/CBB patterns, it has been shown that metal oxide powders can be identified without using the other analytical data such as X-ray diffraction patterns or specific surface area, and similarity/differentness of a pair of metal-oxide samples can be quantitatively evaluated as degree of coincidence of ERDT/CBB patterns. In this talk, a novel approach of material design based on the ERDT/CBB patterns is introduced.

#### Audience Take Away:

- Possible “identification” of solid inorganic materials such as catalysts and photocatalysts by ERDT/CBB patterns measured using reversed double-beam photoacoustic spectroscopy
- Possible extension of ERDT/CBB-pattern study to characterization of amorphous solids and interparticle electronic contact

#### Biography:

The research work on photocatalysis by Professor Bunsho Ohtani started in 1981 when he was a Ph. D. course student in Kyoto University. Since then he has been studying photocatalysis and related topics for 40 years and published more than 300 original papers (h-index: 70) and two single-author books. After gaining his Ph. D. degree from Kyoto University in 1985, he became an assistant professor in the university. In 1996, he was promoted to an associate professor in Graduate School of Science, Hokkaido University and was then awarded a full professor position in the Catalysis Research Center (presently Institute for Catalysis), Hokkaido University in 1998. He was awarded several times from the societies related to chemistry, photochemistry, electrochemistry and catalysis chemistry.





**Matteo Tonezzer\*, Franco Biasioli, Flavia Gasperi**

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## Nanowires in a thermal gradient: From resistive chemosensors to smart detection

Resistive sensors based on metal oxide nanostructures are very interesting because they are tiny, simple, cheap to fabricate and to use, possibly low power consuming, and can sense almost any gas. Unfortunately, this last property is not so positive, because it means that these solid state sensors completely lack selectivity. This comes from the fact that their response is one-dimensional, a dimensionless ratio that indicates at most whether the gas is oxidizing or reducing. This negative aspect can be circumvented by combining the response in different conditions (for example at different working temperatures) so as to get more significant information. Indeed, combining  $N$  sensors working at different temperatures, we obtain an  $N$ -dimensional point that contains the information of  $N$  raw responses, but also the  $N*(N-1)/2$  correlations between the responses themselves. Besides usual PCA visualization, this information can be used in different ways to achieve real smart detection: RGB coding gives a qualitative and semi-quantitative response (similar to a litmus paper), while machine learning algorithms make the system able to recognize the gas and estimate its concentration in a quantitative way. Both of these approaches make it possible to achieve a perfect classification of the gases tested and a very low error on the concentration estimate (5-15%), bridging the gap between simple resistive sensors and electronic noses. Tiny electronic noses that can be integrated into portable devices such as a smart phone are the first step towards a widespread network that will allow to monitor the quality of the air breathed by people and at the same time their health.

### Audience Take Away:

- This contribution will show how to realize tiny electronic noses using metal oxide nanowires
- The use of a thermal gradient (temporal or spatial) can give selectivity to a single nanomaterial
- Different architectures to apply this novel method will be presented
- This transversal approach can be applied in any field, because the semiconducting nanowires have almost no intrinsic selectivity towards specific gases

### Biography:

Matteo Tonezzer received his PhD degree from the Faculty of Physics at the University of Trento, Italy. In 2011, he won the Young Scientist Award from the European Materials Research Society (EMRS). He worked in research centers in France (ESRF), Brazil (UFMG), Vietnam (HUST), Italy (INFM, CNR), South Korea (INHA) and USA (GeorgiaTech). He is currently working for IMEM at the Italian National Research Council. His main area of interest concern the sensing properties of nanostructured organic and inorganic materials and the use of machine learning towards smart sensing.



**Osman Adiguzel**

Department of Physics, Firat University, Elazig, Turkey

## The role of thermomechanical reactions in memory behavior of shape memory alloys

Shape memory effect is a peculiar property exhibited by a series of alloy systems in the  $\beta$ -phase fields. These alloys have dual characteristics called thermoelasticity and superelasticity, governed by successive thermal and stress induced martensitic transformations, and performed thermally and mechanically. Thermal induced transformation occurs along with lattice twinning on cooling and ordered parent phase structures turn into twinned martensite structures. Twinned martensite structures turn into detwinned martensite structures by means of stress induced transformation with deformation. Strain energy is stored in the material with deformation and released upon heating, by recovering the original shape in bulk level, and cycles between original and deformed shapes on heating and cooling, respectively. Superelasticity is also a result of stress induced martensitic transformation and performed by mechanically stressing and releasing at a constant temperature in the parent austenite phase region. The ordered parent phase structures turn into the detwinned structures by means of stress induced martensitic transformation, by stressing. Shape memory effect is performed thermally in a temperature interval depending on the forward and reverse transformation, on cooling and heating, respectively, and this behavior is called thermoelasticity. Thermal induced martensitic transformation occurs as martensite variants with the cooperative movement of atoms in  $\langle 110 \rangle$ -type directions on  $\{110\}$ -type close packed planes of austenite matrix, by means of shear-like mechanism. The  $\{110\}$ - plane family represent 6 planes, and totally 24 martensite variants occur.

Copper based alloys exhibit this property in metastable  $\beta$ -phase region, which has bcc-based structures. Lattice invariant shears are not uniform in copper-based shape memory alloys, and the ordered parent phase structures martensitically undergo the non-conventional complex layered structures on further cooling. The long-period layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice. In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns exhibit super lattice reflections inherited from parent phase due to the diffusion less character of martensitic transformation. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature, and this result refers to a new transformation in diffusive manner.

### Audience Take Away:

- Shape memory effect is a multidisciplinary phenomenon. Shape memory alloys are multifunctional materials and used as shape memory devices from biomedical to the aeronautical and every field of the industry. This phenomenon is based on microstructural changes in the materials

## **Biography:**

Dr 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 on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University, Elazig, Turkey in 1980. He became professor in 1996, and he has been retired due to the age limit of 67, following academic life of 45 years. He published over 80 papers in international and national journals; He joined over 100 conferences and symposia in international and national level as participant, invited speaker or keynote speaker with contributions of oral or poster. He served the program chair or conference chair/co-chair in some of these activities. In particular, he joined in last seven years (2014 - 2020) over 80 conferences as Keynote Speaker and Conference Co-Chair organized by different companies. He supervised 5 PhD- theses and 3 M.Sc- theses.

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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**Jeasmin Akter\*, Md. Abu Hanif, Md. Akherul Islam, Insup Lee,  
Jae Ryang Hahn**

Department of Chemistry, Jeonbuk National University, Jeonju 54896, Korea

## **Enhanced activity of TiO<sub>2</sub>-based photocatalyst under visible light: Selective Preparation of Ti<sup>3+</sup>/TiO<sub>2</sub>/CNT and Ti<sup>3+</sup>/TiO<sub>2</sub>/carbon layer nanocomposites**

TiO<sub>2</sub> is an effective photocatalyst; however, its wide bandgap limits its usefulness to the UV region. As a solution to this problem, a convenient route was developed for the selective preparation of two stable nanocomposites, Ti<sup>3+</sup>/TiO<sub>2</sub>/CNT and Ti<sup>3+</sup>/TiO<sub>2</sub>/carbon layer, from the same precursor by varying the amount of single-walled carbon nanotubes (SWCNTs) used in the synthesis. The nanocomposites exhibit a small bandgap and wide visible light (VL) absorption because of the introduction of carbonaceous species and Ti<sup>3+</sup> vacancies. The nanocomposites exhibit excellent photocatalytic activity toward methylene blue, methyl orange, rhodamine B, and congo red dyes within 25 min. Also, the activity for colorless organic pollutant phenol degradation was tested and found very good activity. Higher reusability and structural integrity of the as-synthesized photocatalyst were confirmed within five consecutive runs by photocatalytic test and X-ray diffraction analysis, respectively. The resulting nanocomposites provide new insights into the development of VL-active and stable photocatalysts with high efficiencies.

### **Audience Take Away:**

- Selective preparation of Ti<sup>3+</sup>/TiO<sub>2</sub>/CNT and Ti<sup>3+</sup>/TiO<sub>2</sub>/carbon layer nanocomposites and their excellent photocatalytic efficiency under visible light
- The described method overcomes the shortcomings of TiO<sub>2</sub> as a photocatalyst under visible light.
- The resulting nanocomposites provide new insights into the development of visible light-active and stable photocatalysts with high efficiencies.

### **Biography:**

Jeasmin Akter is a Ph.D. student in the Department of Chemistry, Jeonbuk National University, South Korea. Her research area is 'Photocatalytic Degradation of organic pollutants and Nanomaterial Synthesis'. She completed her BSc (Hons) and MSc in Chemistry from the University of Rajshahi. She has published her research work in highly reputed journals such as Nature Scientific Report, Mater. Sci. Semicond. Process, ACS-Applied Nanomaterials, Applied Surface Sciences, and J. of Photochem. Photobiol. A, Nanomaterials, and so on.



**Tomasz Borowski\*, Dawid Sołoducha, Rafał Rakoczy, Marian Kordas**

Department of Chemical and Process Engineering, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Piastów Avenue 42, 71-065 Szczecin, Poland

## Studies of influence of a magnetic field on mixing efficiency

Static or alternating magnetic fields may be used to increase the process intensity instead of the mechanical mixing. Static magnetic fields are used as electromagnetic brakes and alternating magnetic fields are commonly used as electromagnetic stirrers. For example, the rotating magnetic field may be used as a non-intrusive stirring device and it can be engineered to provide any desired pattern of stirring. The main aim of this study is to present the results of an experimental analysis of the mixing process under the action of the various types of magnetic fields. Dimensionless correlations are proposed to describe the hydrodynamic conditions in the analyzed mixing system. The results showed that the mixing behavior of the magnetically assisted mixers may be described by means of the term defining the mixing efficiency.

### Audience Take Away:

- Audience will be able to learn about mixing process in magnetically assisted mixers
- This work contains information about using dimensionless analysis to describe the mixing process with the application of magnetic field
- Audience will be able to learn about the application of mathematical description to define the magnetically assisted mixing process

### Biography:

Tomasz Borowski finished his bachelors studies on West Pomeranian University of Technology in Szczecin in 2021, and he is continuing his education on Masters Studies. Since 2018 He is a member of research group led by Prof. Rafał Rakoczy.



**Kamila Splinter\*, Zofia Lendzion Bielun**

Department of Inorganic Chemical Technology and Environment Engineering,  
Faculty of Chemical Technology and Engineering, West Pomeranian University  
of Technology in Szczecin, Szczecin, West Pomeranian Voivodeship, Poland

## **Preparation of Iron pigments based on waste Iron(II) Sulfate**

The study on the possibility of the synthesis of iron pigments based on a waste iron(II) sulfate from the production of titanium dioxide by the Sulfate Process in Grupa Azoty Zakłady Chemiczne "POLICE" S.A.

The work uses solid wastes from the 1980s, which have not been used so far. The purification process of the raw material was carried out, which allowed getting rid of impurities from iron(II) sulfate. The salt purified in this way was the starting material for the synthesis of iron pigments. The synthesis was carried out by two methods - the precipitation method and the precipitation method with the use of a microwave reactor. Iron(III) oxide (red) and iron(III) hydroxide (yellow) pigments were synthesized. Instrumental analytic methods tested the obtained pigments, eg. X-ray Diffraction, FT-IR, or BET surface area analysis. The pigments were analyzed toward color and determination of the oil number as well.

The results showed a change in physicochemical properties depending on the conditions and method of synthesis. Moreover, the similarity of the synthesized pigments to commercial pigments obtained from pure ingredients was found.

Based on the obtained research results, it can be considered that waste iron(II) sulfate may be a potential raw material for the production of iron pigments.

### **Audience Take Away:**

- Possible way to use solid waste iron(II) sulfate
- Characterization of iron pigments based on waste iron(II) sulfate
- Possible use of iron pigments
- How waste management can improve chemical engineering?

### **Biography:**

B. Eng. Kamila Splinter is studying Chemical Technology at the West Pomeranian University of Technology in Szczecin. Since beginning of hers studies, she taking part in research about waste management – she presented her works at conferences for young scientist in Poland, UAE and Portugal. She graduated as B. Eng. in February 2021.



**Swati\*, N. Viswanadham, Umesh Kumar**

CSIR-Indian Institute of Petroleum, Dehradun, India

## **ZSM-5 modified catalysts for the conversion of bioethanol to aromatics**

The production of aromatics and other petrochemicals from renewable sources will be a sustainable approach and reduce the loads on fossil resources. Eventually, it will help reduce the emission of greenhouse gases produced with these materials' combustion. In this work, catalytic conversion of bioethanol to aromatics (BTX) has been studied using modified ZSM-5 catalysts. The modified ZSM-5 catalysts were prepared by the impregnation of transition metals with the variable metal concentration. The detailed characterizations of the prepared catalysts were performed by using Nitrogen physisorption, X-ray Diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Temperature programmed desorption (NH<sub>3</sub>-TPD), Thermal gravimetric analysis (TGA), Scanning electron microscopy (SEM), and Transmission electron microscopy (TEM) techniques. The role of acidity and structure of modified ZSM-5 for the conversion of bioethanol to aromatics has been investigated. The reaction conditions were optimized for the production of aromatics from bioethanol at different reaction parameters, temperature (200-600 °C), LHSV (2-8 h<sup>-1</sup>). At optimum reaction conditions, the catalyst shows 35% BTX selectivity.

### **Audience Take Away:**

- The audience will understand how renewable resources can be used for the production of value-added products.
- The audience will also understand the Zeolites' catalytic properties (ZSM-5) responsible for the conversion of ethanol to aromatics.

### **Biography:**

Swati has completed Masters in Organic Chemistry and is a PhD student in Chemical and Material Sciences Division at CSIR-Indian Institute of Petroleum in Dehradun, India. Her field of interest are catalysis, conversion of bioethanol into value added products.



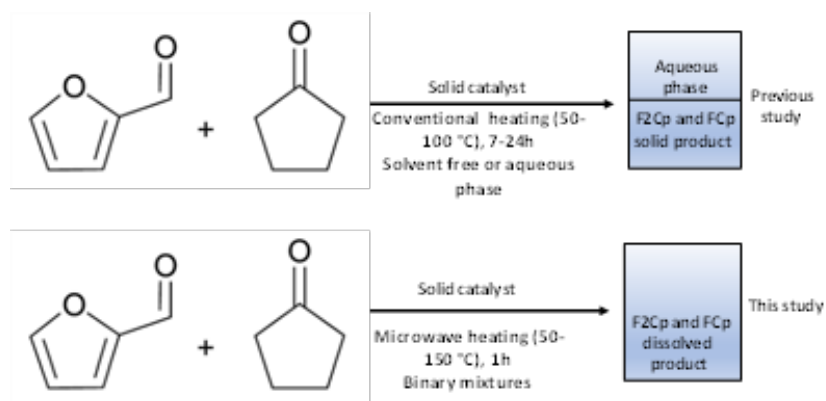


**Richard Ahorsu\*, Dr Magda Constanti, Dr Francisco Medina**

Departament d'Enginyeria Quimica, Universitat Rovira i Virgili, Tarragona, Spain

## Production of liquid fuel from furan derivatives through microwave-aided process in bi-mixtures with monophasic configuration

Concern over global climate change has spurred the development of new pathways for using biomass waste as a raw source for biofuels and commercial chemicals. The utilization of furfural and ketones as feedstocks for aldol condensation and dehydration/hydrogenation to synthesize diesel or jet fuel range alkanes over a solid base or homogenous catalyst was proposed to address dwindling petroleum sources, greenhouse impact, and environmental damage. The use of aqueous NaOH solution as a homogeneous catalyst in aldol condensation reactions causes issues such as catalyst recovery and reaction vessel corrosion. Aqueous phase heterogeneously catalyzed aldol condensation poses unique challenges such as altered reaction processes, increased catalyst leaching, and insoluble products. Performing the process in the presence of green organic solvents could help overcome these issues. In this study, we use bio-based green solvents (ethanol and water: solvent phase reaction) and reactants to produce 2,5-bis(2-furylmethylidene) cyclopentanone (F2Cp) and 2-(2-furylmethylidene) cyclopentanone (FCp). In order to minimize reaction time and boost product yield, microwave (MW) aided procedures coupled with Mg-Zr mixed oxide was used. We achieved a global yield of ca. 34 % in 60 min of reaction and a considerable FCp and F2Cp global yield after 4 runs of recovered catalyst.



**Graphical Abstract**

### Audience Take Away:

- It is expected that, this presentation will demonstrate to audience the advantages of using green solvent in reaction to prevent catalyst deactivation.
- Integrating microwave processes into biorefineries for the consolidation of green process
- Current state of utilization of furan derivatives for the production bio jet fuel precursors

**Biography:**

Richard Ahorsu is a PhD candidate in Nanoscience, Materials and Chemical Engineering at Rovira I Virgili University in Tarragona, Spain. He also holds a master's degree in Nanoscience, Materials, and Chemical Technology from the same university. He joined Dr Roberto Rinaldi's Tomorrow's Chemical Technologies Lab at Imperial College London as a visiting doctoral student in 2019. He specializes in green chemistry, heterogeneous catalysis, and fermentation (bio-catalysis). He has published in peer-reviewed journals.



**Olga Bartlewicz\*, Mariusz Pietrowski, Hieronim Maciejewski**

Poznań Science and Technology Park, Adam Mickiewicz University  
Foundation, Rubież 46, Poznań, 61-612, Poland  
Adam Mickiewicz University in Poznań, Chemistry Department, Uniwersytetu  
Poznańskiego 8, 61-614 Poznań

## **SILP materials based on $\text{TiO}_2$ - $\text{SiO}_2$ support as efficient and recyclable catalytic systems for hydrosilylation reaction**

Catalytic processes are one of the most important branches of the chemistry. Heterogeneous catalysts which reduce the costs of the reaction and enable their easy isolation and reuse, are very important aspects of this field. One of the more and more used heterogenization method of homogeneous catalysts is application of Supported Ionic Liquid Phase (SILP) systems. Preparation of SILP materials containing metals or metal complexes is carried out by immobilizing the active substance on the surface of a porous support, covered with a thin layer of ionic liquid. This method allows to increase catalysts stability and durability. Hence, obtained materials are used in many chemical reactions, e.g. in hydrosilylation processes. It is worth noting that in SILP systems very often silica materials are used as a support and hybrid oxide systems, such as  $\text{TiO}_2$ - $\text{SiO}_2$ , have not already been used in this type of catalytic systems. The hydrosilylation reaction is one of the leading methods of obtaining silicone products, such as rubbers, sealants, adhesives or modified polymers. This reaction also enables the production of organofunctional silicones, which due to the introduction of functional groups into their structures are chemically reactive. The hydrosilylation process is a catalytic reaction, mainly catalysed by homogeneous transition metal complexes. Therefore, due to the economic and ecological aspects of the above process, it is important to use heterogeneous catalytic systems, that enable easy isolation and reuse in subsequent catalytic cycles. The presented research results refer to new SILP systems with  $\text{TiO}_2$ - $\text{SiO}_2$  materials. In the conducted research also the influence of the structure of the support and applied ionic liquid on the catalytic efficiency in the hydrosilylation reaction was examined. Prepared materials were subjected to extensive physicochemical and adsorption analysis.

### **Audience Take Away:**

- The presented new Rh-SILP and Pt-SILP materials may be an interesting alternative to popular homogeneous catalysts in many catalytic reactions, especially in the hydrosilylation reaction.
- Combination of at least two different oxides allows to combine unique properties of individual oxides and permits e.g. for enlargement of the surface area of the support.
- The presented research results will provide information on the synthesis and physicochemical properties of both the applied  $\text{TiO}_2$ - $\text{SiO}_2$  support and the SILP systems.
- Heterogenization of the catalytic system by preparing SILP materials positively affects the economic and ecological aspects of the hydrosilylation reaction.

### **Biography:**

MSc. Olga Bartlewicz is a PhD student at the Adam Mickiewicz University in Poznań at Department of Chemistry. Graduate from Poznań University of Technology (Faculty of Chemical Technology). In 2013, she obtained an engineering degree and in 2014 a master's degree in the specialization of Organic Technology. Her scientific interests are related to the catalysis of hydrosilylation reactions with the use of new rhodium and platinum catalysts with ionic liquids as ligands, and also with the use of SILP (Supported Ionic Liquid Phase) systems as heterogeneous catalytic materials in the synthesis of organofunctional siloxanes.

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**Linda Zh Nikoshvili\*, Alexey V Bykov, Liubov Kiwi-Minsker**

Department of Biotechnology, Chemistry and Standardization, Tver State Technical University, Tver, Russia

## **Aromatic polymers as a stabilizing medium for Pd nanoparticles in Suzuki reaction**

**A**mong different polymers nanostructured cross-linked aromatics have the greatest potential as catalytic supports due to their exceptional thermal and chemical stability and preservation of the active phase morphology. Hyper-cross-linked aromatic polymers (HAPs) allow using its microporous structure for stabilization of metal nanoparticles (NPs). In this work we explore the limits of HAPs applicability in Pd-catalyzed cross-coupling reactions by the example of Suzuki reaction. The reaction was carried out in ethanol-water mixture at the absence of phase-transfer agents at variation of the initial palladium oxidation state, reaction temperature, concentrations of the main reagents and aryl halide nature. Experimental data revealed that Pd NPs can be retained in HAP environment during the repeated runs at chosen reaction conditions though the changes in NPs morphology and sizes distribution takes place depending on the initial oxidation state of Pd. Unrestricted DFT calculations at the BP level of theory using triple-zeta basis sets confirmed that aromatic rings can retain small palladium clusters (Pd<sub>4</sub> and Pd<sub>9</sub>). The similar effect can be proposed for small metal NPs. However, the activity of Pd/HAP catalysts is also attributed to the ability of formation of homogeneous Pd species. It is known that several forms of palladium can simultaneously participate in the catalytic cycle of Suzuki reaction: dissolved molecular complexes Pd(0) and Pd(II), colloidal Pd in solution and/or on a support, and large-diameter particles of metallic palladium. Thus, various processes (e.g. aggregation, dissociation, leaching, and etc.) can contribute to changes in the catalyst morphology and, as a result, its activity and selectivity. In this work, we also present our recent DFT calculations, which show that, depending on the halogen type, different aryl halides reveal different types of adsorption on small Pd clusters, which may likely alter the ability to form homogeneous palladium species. Thus different reaction ability of aryl halides can be attributed to their leaching ability of palladium from the ligandless catalysts.

### **Audience Take Away:**

- The presented data will be useful for understanding of the behavior of polymer-based catalysts in cross-coupling reactions.
- From the presented data the limits of applicability of ligandless catalysts based on aromatic polymers in cross-coupling reactions will be clearer.
- The benefits from the use of aromatic polymers as catalytic supports will be obvious.

### **Biography:**

Linda Zh. Nikoshvili graduated the Department of Biotechnology and Chemistry of Tver State Technical University (TSTU) as MS in 2006. She received her PhD degree in Catalysis in 2009. After one year she obtained the position of an Associate Professor at the TSTU. For the achievements in the field of heterogeneous catalysis she received "Honorary diploma of the Ministry of Economic Development of the Tver Region" (2013), the award "Engineer of the Year" (2013) and Honorary diploma of the Governor of the Tver Region (2017). She has published more than 50 research articles in SCI(E) journals.



**Dawid Sołoducha\*, Tomasz Borowski, Rafał Rakoczy, Marian Kordas**

Department of Chemical and Process Engineering, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Piastów Avenue 42, 71-065 Szczecin, Poland

## Neutralization reaction induced by different types of magnetic field

The study investigated the possibility of conducting mixing process in a custom mixing system equipped with a magnetic field generator.

The aim of presented work was to apply magnetic fields (rotating magnetic field, static magnetic field, pulsating magnetic field and oscillating magnetic field) for intensification of neutralization process. The second step was to use the obtained results to the analysis of magnetic fields. Finally, the results were compiled in the form of mathematical relation and compared with each other.

The process of mixing liquids is usually carried out with the use of various types of mixers equipped with a mechanical agitator. In literature one can find various types of mixers, agitators and alternative ways to proceed mixing process, for example using magnetic fields. In presented work it was demonstrated, that some types of magnetic fields may be used to intensify neutralization process by the force of mixing.

The results showed the differences in hydrodynamic of the liquid exposed to the influence of various types of magnetic fields, what means that one can use some of this types in specific mixing setups. Additionally, it is possible to use ferromagnetic ( $\text{Fe}_2\text{O}_3$ ) as a strengthening factor, thanks to which much better mixing properties may be obtained. This specific mixing system may be used in processes of mixing in biotechnology, where microorganisms are exposed to stress connected with specific process of mixing.

### Audience Take Away:

- Audience will be able to learn about new types of magnetic mixers
- This work contains information about using neutralization process in mixing time measuring
- Audience will be able to learn about differences between different types of magnetic field compared to each other

### Biography:

Dawid Sołoducha is a Masters student on West Pomeranian University of Technology in Szczecin. He finished his bachelors studies on West Pomeranian University of Technology in Szczecin in 2021. Since 2018 He is part of research group led by Prof. Rafał Rakoczy,



**Mahdi Bourassi\*, Gwendoline Lafaye, Jana Gaalova, Jacques Barbier J**

Institut de Chimie des Milieux et Matériaux de Poitiers, Poitiers university, Poitiers, France

Institute of Chemical Process Fundamentals, Czech Academy of Science, Prague, Czech Republic

Environment Science Institute, Charles University, Prague, Czech Republic

## **Catalytic wet air oxidation of antibiotics over supported Platinum on different supports fractions based CeO<sub>2</sub> and ZrO<sub>2</sub>**

Emerging contaminants have serious effects on the environment. Especially contaminants loaded with used water, which affect fauna, flora, and contaminate soils. Antibiotics are considered as an emerged threat originated from leaking and incompletely treated wastewater loaded with pharmaceuticals. Antibiotics risks are divers, the most pertinent are environment useful microorganism deterioration and harmful bacteria gaining antibiotics resistance. Those factors could generate in the future sanitary and environmental crisis. Facing these issues, many technologies propose sufficient solutions to release only cleaned water, as example, adsorbents and membrane separations, which have successful separation results. The only issue is these separation methods generate highly contaminated solutions or adsorbents, which are even more threatening and extremely hard to handle. Catalytic Wet Air Oxidation (CWAO) is one of the most efficient concentrated wastewater detoxification processes.

We have investigated catalytic oxidation of model antibiotics solutions, mainly based tetracycline for their excessive uses and presence in the environment. Different supports (Ce, Zr) and Pt-based catalysts supported on these oxides were tested at two different degradation temperatures and compared, including the blank catalyst-less: wet air oxidation. Periodically collected liquid samples were characterized using different methods: HPLC-UV and TOC-L analysis to follow the conversion of the model pollutant and quantification of total organic carbon, also HPLC-MS for by-products identifications. Concerning fresh and used catalyst characterization, we have implemented an ICP analysis for noble metal quantification and leaching investigation, specific surface characterization, and TEM analysis. All the analyses carried out have contributed to the interpretation of the results and to prove the explanations. The catalyst effect on catalytic wet air oxidation tests are very significant. For example, at 50°C atmospheric pressure Pt/CeZr showed the best activity, reaching 98%  $\Delta$ [TOC]%, and even more the selectivity SCO<sub>2</sub>% index was 100% during all three hours of CWAO, as well at room temperature catalysts still present good degradation results. Moreover, collected samples by-products are identified, and treated solutions toxicity are inspected.

### **Audience Take Away:**

- Membrane separations processes are not complete water treatments. They generate concentrated by-product which are more dangerous, further treatment for those solutions is required
- For full pharmaceutical wastewater treatment, hybrid treatment like membrane separation followed with an advanced oxidation process is recommended for persistent compound degradation
- Catalytic wet Air Oxidation is an effective process for highly contaminant loaded wastewater
- The hybrid processes are to be applied directly after concerned industries which generate persistent contaminants. This will prevent from environment deterioration and bacterial resistant development
- Catalytic Wait Air Oxidation process must releases only harmless biodegradable wastewater which can be proceeded to conventional treatments or even released into the environment

**Biography:**

Mahdi Bourassi Graduated with a MSc. fundamental chemistry, in 2018, from the Chouib Doukali University, El Jadida, Morocco, after completing an internship at University of Oulu, Finland. Now he is a PhD student at the Environmental Science Institute, Charles University, Prague. He also works at the Institute of Chemical Process Fundamentals, Department of Membrane Separation Processes, as a research assistant. He set up a fellowship with Poitiers University, France, to expand his research on elimination of drugs from water through hybrid process, membrane separation followed by Catalytic Wet Air Oxidation processes, he is a member of the MELEV project.





**Bouaziz Lydia\*, SI-Ahmed Kahina, Bessekhoud Yassine**

Laboratory of Functional Organic Analysis, Faculty of Chemistry, Algeria  
Laboratory of Storage and Valorization of Renewable Energies, Faculty of  
Chemistry, Algeria

## Effect of Iodine doping ZnO on electrochemical ethylparaben (EthP) detection

Parabens, esters of p-hydroxybenzoic acid (including methylparaben (MeP), ethylparaben (EthP), propylparaben (PrP) and butylparaben (BuP)), are homologous molecules used in industry due to their antimicrobial activity. These molecules are also present naturally in many ecosystems. Parabens are well known to be endocrine disruptors. Accordingly, it is of prime importance to control their concentration in the food industry, cleaning products, pharmaceutical products, and cosmetics products. The present study focuses on developing a new material electrode that serves as a parabens detector in the electrochemical process. In this context, Zinc Oxide "ZnO" was doped with iodine at various levels to improve its physicochemical properties.  $I_x\text{ZnO}$  ( $x=0.000, 0.025, 0.05, 0.075$  and  $0.1$ ) nanoparticles were prepared by microwave-assisted method and characterized by XRD, XPS, SEM, and DRS. A deep electrochemical characterization including cyclic voltammetry, Tafel plots, Mott-Schottky measurements, and Electrochemical Impedance Spectroscopy (EIS) has been adopted. All these techniques served the investigation of the feasibility of ethylparaben (EthP) detection. The oxidation of EthP was studied in the concentration range of 10 mM to 0.08 mM. A characteristic peak of anodic oxidation was observed at a potential of 0.767V vs. ECS. The best electrochemical EthP sensing process was obtained using  $I_{0.1}\text{ZnO}$  electrode with a detection limit (DL) and a quantification limit (QL) of 0.0405 mM and 0.1351 mM, respectively. The proposed sensor showed a high-efficiency detection of EthP in cosmetics. The obtained results were corroborated with those obtained with HPLC.

### Audience Take Away:

- The audience will learn how to perform anionic doping of ZnO with iodine.
- The audience will learn how iodine doping modifies the structural and electrochemical properties of ZnO.
- The audience will learn how iodine doping improves paraben (EthP) detection with high efficiency.
- This work opens new opportunities in the field of anionic doping of ZnO.
- The audience will appreciate the different electrochemical techniques used in this work and how the data are deduced.
- The audience will understand the relationship between the novel properties induced by doping and the detection capacity of parabens.
- This work can serve as a model of work in the field of electrochemical detection.
- This work can teach electrochemical methods and as a base in the case of research according to the methodology used and the relevant results obtained.
- This work provides innovative materials and an analytical method for easy and fast parabens detection with low cost compared to the classical method using HPLC.

**Biography:**

BOUAZIZ Lydia is currently a Ph.D at the university of Sciences and Tchnology Houari Boumediene (U.S.T.B.). She received his master degree in analytical chemistry (2017) from U.S.T.H.B. The main areas of areas of research are the environmental (sensors and photocatalytic) applications, forensic applications and biological interest using electrochemical and analytical methods.



**Jelena Petrovic\*, Marija Simic, Marija Mihajlovic, Marija Koprivica, Jelena Dimitrijevic**

Institute for Technology of Nuclear and Other Raw Mineral Materials, Belgrade, Serbia

## **Efficient adsorption of lead ions from aqueous solution using Fe/Mg modified grape pomace hydrochar**

Within this study, the potential application of grape pomace hydrochar as a potential adsorbent of lead ions from aqueous solutions will be investigated for the first time. For preparation of hydrochar, the grape pomace was hydrothermally carbonized in aqueous medium at 220 °C within 1 h. Obtained material was further modified with Mg and Fe salts in order to improve its adsorption properties. Preliminary adsorption results showed that the modified hydrochar exhibited significantly higher adsorption capacity (139.5 mg g<sup>-1</sup>) compared to the unmodified one (27.8 mg g<sup>-1</sup>). Further examination of the effects of different adsorption parameters (initial pH value and contact time) using modified and unmodified hydrochar, defined their optimum values for the most effective lead removal. The obtained results showed that the most efficient removal of lead ions occurs in solutions with pH 5. Furthermore, the examination of the influence of time on the adsorption process demonstrated that in the beginning the adsorption takes place quickly. The reason for this is the large number of available active centres on the hydrochar surface that can bind lead ions. However, as the number of these centres is occupied by a longer contact time, the binding rate decreases and after 240 minutes the equilibrium is reached. Kinetic models of pseudo-first and pseudo-second order were applied to the results of the influence of contact time. The kinetic study implied that the removal of lead ions on modified hydrochars follows pseudo-second order model. This model assumes a chemical interaction between lead ions and groups on the surface of hydrochar as the main binding mechanism. Based on the above it can be concluded that the hydrothermal carbonization is very efficient technology for conversion of waste biomass into highly valuable products. In order to examine in more detail the binding mechanism and the process of metal adsorption using modified hydrochars, additional analyzes will be part of our future research.

### **Audience Take Away:**

- Hydrothermal carbonization as perspective process for waste agricultural residue, grape pomace, valorization.
- Examination of chemical modification of the hydrochars surface by Fe and Mg salts in order to improve ability of obtained material to remove pollutants from wastewater
- Mechanism and surface interaction between material and selected pollutant
- The results of this study contribute to the development of a new technology for obtaining value-added products from waste grape pomace, while ensuring sustainable management of waste biomass and closing the product life cycle.

### **Biography:**

Jelena Petrovic, finished MS studies at the Faculty of Natural Sciences and Mathematics, University of Novi Sad in 2011. Doctoral studies at the Faculty of Technology and Metallurgy, University of Belgrade she ended in 2017. Since 2013., Jelena Petrović has been employed at the Institute for Technology of Nuclear and Other Raw Mineral Materials. Her investigations are based on the implementation and optimization of the hydrothermal carbonization process in order to valorize the agricultural residues into value-added products. As an author or coauthor, she published over 80 publications in the form of scientific papers and conferences.



**Bhavana B. Kulkarni\*, Kempanna S. Kanakikodi, Sanjeev P. Maradur**

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Graduate studies, Manipal Academy of Higher Education, Manipal -576104, Karnataka, India

### **One-pot hydrogenation-esterification of furfural with acetic acid for the selective synthesis of furfuryl acetate over bifunctional Pd@UiO-66(Hf) catalyst**

Development of new strategies for tandem reactions that demands composite catalyst with multifunctionality is essential for bio-oil upgradation. This work focuses on a model bio-oil-upgrading method, one-pot hydrogenation-esterification (OHE) of furfural with acetic acid for the selective synthesis of furfuryl acetate using a bifunctional Pd@UiO-66(Hf) core-shell material. For comparison, the catalytic performance of support material [Pd/UiO-66(Hf)] synthesized by simple impregnation method was studied in the OHE reaction. The physicochemical properties of the materials have been systematically studied by employing various characterization techniques. Here, the high-synergistic effect of Brønsted acidic sites over SBU (Secondary building unit) of MOF and Pd NPs (Nanoparticles) in the core-shell material over Pd/UiO-66(Hf) is reflected in terms of the catalytic activity of the materials. The core-shell material demonstrated high catalytic activity with 56.6% yield of furfuryl acetate as compared to Pd/UiO-66(Hf) hybrid material (38.7% yield). The excellent performance exhibited by Pd@UiO-66(Hf) outperformed the reported materials for this transformation. This avenue opens up the opportunities for the efficient transformation of bio-derived molecules into value-added products using bifunctional hybrid materials.



**Binitha N Narayanan\*, Sudha Kochiyil Cherikkallinmel**

Department of Chemistry, Sree Neelakanta Government Sanskrit College  
Pattambi (Affiliated to University of Calicut), Palakkad-679306, Kerala, India

## Highly reusable novel Sodium Titanate nanotube catalyst for biodiesel production

Being renewable and clean-burning, biodiesel, originated from triglyceride oils/fats, get relevance over conventional diesel fuels. Among the different triglyceride sources, waste cooking oil has high significance in terms of price and effective use of waste material. Highly reusable sodium titanate nanotube catalyst is developed here from porous titania and NaOH via wet impregnation method for its catalytic application in biodiesel production by the transesterification of waste cooking oil with methanol. Here, NaOH is incorporated into the porous sol-gel derived  $\text{TiO}_2$  prepared in the presence of a nonionic surfactant in an aqueous solvent. The X-ray diffraction pattern of the catalyst indicated  $\text{Na}_2\text{Ti}_3\text{O}_7$  as the active crystalline phase of the material responsible for catalysis. XPS analysis confirmed the formation of  $\text{Na}_2\text{Ti}_3\text{O}_7$ , whereas TEM analysis revealed the porous nanotubular morphology. Investigation of the effect of reaction variables on catalytic performance indicated the viability of the catalyst in a range of mild reaction conditions. The catalyst showed excellent activity and gave a fatty acid methyl ester content of 100% under the selected reaction conditions of catalyst weight of 4 wt% of oil, methanol/oil molar ratio of 15:1 at the reaction temperature of 65 °C for 1.5 h reaction. Catalyst leaching and loss of activity in repeated cycles are one of the most inevitable hurdles in biodiesel catalysts, but here, no loss in the activity was detected even up to five repeated cycles of catalysis, demonstrating the efficiency and stability of the present catalyst. The prepared biodiesel met the various specifications stated in the biodiesel standard, mainly United States biodiesel standard ASTM D6751 and European biodiesel standard EN14214, claiming its safe use as fuel in diesel engines.

### Audience Take Away:

- A highly efficient catalyst is presented here for the preparation of biodiesel, the clean-burning renewable fuel.
- Catalyst preparation and their performance on the specific reaction is of high relevance, and here is a demonstration of catalyst architecture for efficient catalysis with the use of a non-ionic surfactant that improved the incorporation of active species. This can be effectively used for the large-scale production of biodiesel. High reusability is the additional attraction.

### Biography:

Dr. Binitha N Narayanan studied Chemistry at the Cochin University of Science and Technology, India and graduated with as MSc in Applied Chemistry in 2001. She then joined the research group of Prof. Sugunan at the Department of Applied Chemistry, Cochin University of Science and Technology, Kochi, India. She received her PhD degree in 2007 at the same institution. She joined as Assistant Professor in Chemistry at Sree Neelakanta Govt. Sanskrit College Pattambi in 2006 and meanwhile had done one-year postdoctoral fellowship (2008-2009) supervised by Prof. Dr Zahira Yaakob at the Department of Chemical and Process Engineering, National University of Malaysia, Malaysia. She has published more than 60 research articles in SCI(E) journals.



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## The role of the hydrolases in drug synthesis

Enzymes are molecules in most protein structures that catalyze important biochemical reactions in living organisms. But in the early 2000s, studies have shown that enzymes can also be used in drug synthesis. Chemical syntheses may damage the environment, require the use of chemicals that are expensive and potentially toxic to living organisms, often require additional steps for purification, and obtaining the desired enantiomers in these syntheses is difficult. For these reasons, researchers tended to use chemoenzymatic drug syntheses that are environmentally friendly, effective, efficient, and reusable. Enzymes are used in these syntheses. Hydrolase enzymes are one of the enzymes that are often used in drug synthesis. Hydrolases are enzymes that catalyze hydrolysis reactions. They are commonly used to obtain enantiomerically pure drug precursors in drug synthesis.

Lipases were used in the synthesis of pregabalin which is an anticonvulsant drug, tryptase inhibitors, 15-deoxyspergualin which is an immunosuppressive agent, rasagiline used in the treatment of Parkinson disease, duloxetine which is an antidepressant drug, ibuprofen, ketoprofen, and naproxen which are nonsteroidal anti-inflammatory drugs and doxazosin which is an  $\alpha 1$  – selective adrenergic antagonist. Esterases were used in the synthesis of doxazosin which is an  $\alpha 1$  – selective adrenergic antagonist and glycosidases were used in the synthesis of rare ginsenosides. Epoxide hydrolases were used in the synthesis of propranolol which is a beta antagonist and linezolid which is an antibiotic. Peptidases were used in the synthesis of proteasome inhibitors, (+)-gamma-lactamases were used in the synthesis of abacavir which is an antiviral drug, and nitrilases were used in the synthesis of nicotinic acid. In addition, the importance and the advantages of chemoenzymatic syntheses, reactions catalyzed by these enzymes, results of synthesis, and the general information about used hydrolase enzymes were investigated in detail.

### Audience Take Away:

- The audience will learn about some hydrolase enzymes that play a critical role in the enzymatic synthesis of various drugs and drug precursors.
- There may be an alternative synthesis route that can be applied in the laboratory to the person working in the synthesis of drugs and drug-derived compounds.
- It may be an important opportunity for her/him to recognize hydrolase enzymes.
- She/He can use this knowledge both theoretically and practically.
- Due to its catalytic importance, it may be causing the investigation of new types of hydrolase enzymes.

### Biography:

Dr. Alptekin studied the Department of Chemistry at the Cukurova University, Turkey and graduated as MS in 2003. She received her PhD degree in 2009 at the same institution. After four years she obtained the position of Assist Professor at the Faculty of Pharmacy at Cukurova University. She has published more than 14 research articles in SCI(E) journals and 530 over cites.



**Riheb Mabrouk\*, Hassane Naji, Hacen Dhahri**

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## **Advanced Lattice Boltzmann simulation of melting/solidifying processes of a composite metal foam/paraffin through a rectangular channel**

This work performs a numerical investigation of time-dependent forced convection heat transfer in a rectangular open-ended channel fully filled with a porous structure (metal foam) and saturated with a phase change material (PCM) which is the paraffin. The unsteady two-dimensional governing equations, based on the Darcy-Brinkmann-Forchheimer (DBF) model for the dynamic field and the local thermal non-equilibrium (LTNE) condition for the thermal field at the representative elementary volume (REV) scale in their dimensionless forms, have been simulated using the thermal Single Relaxation Time (T-SRT) Lattice Boltzmann Method (LBM). Three distribution functions are used to handle the fluid, and temperature of both fluid and solid phases. A comparison with previous results in literature is done to validate the in-house code and prove its reliability. Effects of Reynolds number, Eckert number, porosity and pore density on dynamic and thermal fields, entropy generation, Bejan number and energy and exergy efficiencies of the system deemed are analyzed. The relevance of these parameters is highlighted and discussed during the charging (melting) and discharging (solidifying) cycles. Based on the results obtained, it can be stated that low porosity values (0.4 and 0.6) promptly speed up these two processes owing to high thermal conductivity of the metal foam and then, enhance energy and exergy efficiencies of the device, whatever Re. Besides, streamlines, isotherms and melt front (phase field) are presented. In addition, it can be concluded that there is a critical Reynolds number (around 400) for which the quantity of the storage energy is optimal and whose quality is large depending on both the porosity and the viscous dissipation effects.

### **Audience Take Away:**

The investigation keeps focus on latent heat storage in porous duct fully filled with a phase change material (PCM). The aims of this work is

- Analyzed the parameters that influence the system
- found the optimum physical conditions in order to obtain the maximum of stored energy
- calculated the thermal performances of the system

### **Biography:**

Riheb Mabrouk did a preparatory cycle at the Higher Institute of Applied Science and Technology of Gabes. Then she followed her engineering cycle at the national engineering school of Gafsa/ University of Gafsa. Now, she is a PHD student at the National Engineering School of Monastir/ Monastir University. Her research focus on thermal energy storage in porous medium using the Lattice Boltzmann method (LBM). She has published four papers in International Journal of Heat and Mass Transfer, International Communication in Heat and Mass Transfer, energies and processes.





**Md Nurul Islam Siddique**

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## **Impact of supplementary nutrients on Bio-methane production from anaerobic digestion of farming waste: Feasibility & fertilizer recovery**

Unlike wastes digested together might be the enhancement of needs for the micro-organisms drawn in with anaerobic digestion. In the present study, the influence of supplements on the digestion of cultivating substrates was evaluated. An improvement plan which serves a critical job in the anaerobic digestion was used at three stages: 37 °C, 40 °C, and 50 °C. Results showed that at 37 °C by the utilization of enhancements, biogas production accomplished 1.38-times that of control. Additionally, 40 °C without supplements addressed a fascinating philosophy as a result of the incredible utilization of this mid-temperature that had been found huge (56 % of VS end and 8.4 L-biogas). The anaerobic co-digestion at 50 °C exhibited that biogas production surpassed 11.3 L with supplements and that mL-CH<sub>4</sub>/g-VS were 1.24-times that achieved for the system without extra enhancement. Results for each temperature exhibit that the enhancement course of action adds to co-digestion. Also, 37 °C was the most utilized temperature on the advanced scale and had the best impact on the utilization of enhancements during the anaerobic process. Recovery of sludge was 0.09 m<sup>3</sup> sludge/m<sup>3</sup> substrate and the recovery of water was 0.86 (m<sup>3</sup> sludge/m<sup>3</sup> substrate) from the digester. The processed sludge can be utilized as compost and the water can be utilized for irrigation purposes. The time required to recapture the investment was seen as 3.77 y.

### **Audience Take Away:**

- Anaerobic digestion (AD) collects methane and provides a source of renewable energy that is carbon neutral i.e. provides energy with no net increase in atmospheric CO<sub>2</sub>. Fertilizer - compared to undigested slurry, the nitrogen in digestate is more readily available as a plant nutrient.
- Farming waste production around the globe is up to 6 million tons yearly. From these wastes, those that originate from regular trade are yet disposed of in landfills and used for the ignition method with no treatment. This methodology, along these lines, prompts higher GHG emanations and environmental pollution. Anaerobic co-fermentation has been demonstrated to be a successful methodology for improved bio-methane generation from wastes. The mix of different substrates improves nutrition in the digestion system. Thus, microbes have access to supplemented media with an appropriate nutrient equalization. The fundamental targets of co-digestion ought to support valuable associations, keeping away from hindrance and upgrading methane generation. Yes, this research that other faculty could use to expand their research or teaching. Yes, this provides a practical solution to a problem that could simplify or make a designer's job more efficient. Yes, it improves the accuracy of a design or provides new information to assist in a design problem. all other benefits are listed below:
- Improved hydrolysis, pathogen removal, and minimum odor are the key benefits of a thermophilic run.
- On the other hand, the mesophilic run saves energy and is not affected by shock loading than a thermophilic run.
- Besides, a vast microbial community is estimated under a mesophilic state that may help to digest numerous types of organic substances.
- The thermophilic state helps the elimination of pathogens and produces enhanced methane. Nevertheless, the use of intermediate temperatures has not been studied deeply which can influence the system.



- The related works found in the literature didn't study the gap between the feasibility study and fertilizer recovery. Therefore, our work is novel and has detailed data and explanations on the feasibility study and fertilizer recovery.

**Biography:**

Dr. Md Nurul Islam Siddique studied Civil Engineering at the Khulna University of Engineering & Technology, Bangladesh, and graduated as MS in 2012 from University Malaysia Pahang. He then joined the research group of Prof. Zularisam at the Institute of University Malaysia Pahang. He received her Ph.D. degree in 2015 at the same institution. After that, he obtained the position of Assistant Professor at the University Malaysia Pahang. She has published more than 40 research articles in ISI journals.

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