



4<sup>th</sup> Global Summit on

# CATALYSIS & CHEMICAL ENGINEERING

April 13-14, 2023 | Rome, Italy

**Venue:**

Hotel – NH Roma Villa Carpegna,  
Rome, Italy

**Theme:**

“Contemporary Innovations  
and Emerging Novel Research in  
Catalysis and Chemical Engineering”

Chemical Catalyst 2023

<https://catalysis.mindauthors.com/>



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# Scientific Agenda



## Day 1 - Room 1 - Raffaello A

08:00 - 08:30 Onsite Registration &amp; Seating Arrangement

08:30 - 09:00 Introduction &amp; Open Ceremony

## Session 1 - Raffaello A

## Keynote Presentations (Duration: 1hr)

09:00 - 09:30 **Sharmila M. Mukhopadhyay**  
*University of Maine Orono, USA*  
**Hierarchical Biomimetic Nanocatalyst Architectures**

09:30 - 10:00 **Hugo de Lasa**  
*University of Western Ontario, Canada*  
**The CREC Fluidized Riser Simulator a Unique Tool for Catalytic Process Development**

10:00 - 10:20 (Refreshment &amp; Coffee - Duration: 25min)

## Keynote Presentations Cont.. (Duration: 1hr)

10:20 - 10:50 **Alessia Ciogli**  
*Sapienza University of Rome, Italy*  
**Multifaceted use of mass spectrometry in catalysis: from selection of organocatalyst to the investigation of reaction mechanism and related intermediates**

10:50 - 11:20 **Püntener Kurt**  
*F. Hoffmann-La Roche Ltd, Switzerland*  
**Highlights & New Insights in Asymmetric Hydrogenation of Keto (Enol) Esters**

## Session 2 - Raffaello A

## Oral Presentations (Duration: 1hr 40min)

11:20 - 11:45 **Katia Martina**  
*University of Turin, Italy*  
**A highly efficient and sustainable route for nitro benzene reduction with Copper Nanoparticles and Glycerol**

11:45 - 12:10 **Ricardo Rodríguez**  
*CSIC – Universidad de Zaragoza, Spain*  
**Rhodium-Centered Stereogenic Complex with a Tripodal Tetradentate Ligand**

12:10 - 12:35	<b>Alessandro Sacchetti</b> <i>Politecnico di Milano, Italy</i>	<b>Polyethylenimine-based materials: novel heterogeneous catalysts for sustainable organic transformations</b>
12:35 - 13:00	<b>Saim Emin</b> <i>University of Nova Gorica, Slovenia</i>	<b>Sustainable electrocatalytic processes using iron phosphide thin films</b>
<b>Memorable Group Photo &amp; Selfie</b>		
<b>13:00 - 13:45 (Tempting Buffet Lunch - Duration: 45min)</b>		
<b>Session 3 - Raffaello A</b>		
<b>Oral Presentations Cont.. (Duration: 2hr 30min)</b>		
13:45 - 14:10	<b>Juqin Zeng</b> <i>Politecnico di Torino, Italy</i>	<b>Engineering copper nanoparticle electrodes for tunable electrochemical reduction of carbon dioxide</b>
14:10 - 14:35	<b>Elena Pastor</b> <i>University of La Laguna, Spain</i>	<b>Electrocatalysis on carbide and graphene-based materials for electrochemical devices</b>
14:35 - 15:00	<b>Giorgio Della Sala</b> <i>University of Salerno, Italy</i>	<b>Phase-transfer catalysts for sustainable stereoselective synthesis of amino acid and lactone derivatives</b>
15:00 - 15:25	<b>Dario Allevi</b> <i>University of the Sacred Heart, Italy</i>	<b>Gold (I)-catalyzed an efficient and mild synthesis of 3,8-Diarylidene-2,7-dioxaspiro[4.4]nonane-1,6-diones</b>
15:25 - 15:50	<b>Maria Eugenia Rabanal Jimenez</b> <i>Universidad Carlos III de Madrid, Spain</i>	<b>Effect of lithium co-doping on structural, morphological and photocatalytic properties of RE-doped ZnO</b>
15:50 - 16:15	<b>Adalyz Ferreira Fernández</b> <i>University Carlos III of Madrid and IAAB, Spain</i>	<b>Structural and morphological evaluation of Gd-Li co-doped ZnO system with improved photocatalytic activity</b>
<b>16:15 - 16:35 (Refreshment &amp; Coffee - Duration: 20min)</b>		
<b>Session 4 - Raffaello A</b>		
<b>Oral Presentations (Duration: 1hr 40min)</b>		

<p><b>16:35 - 17:00</b></p>	<p><b>Marco Sirignano</b> <i>University of Salerno, Italy</i></p>	<p><b>Synthesis of propiolic acids by silver-catalyzed insertion of CO<sub>2</sub> to terminal alkynes</b></p>
<p><b>17:00 - 17:25</b></p>	<p><b>Yun LI</b> <i>Paris Sorbonne University, France</i></p>	<p><b>Formate Dehydrogenases Mimics as Catalysts for Carbon Dioxide Reduction</b></p>
<p><b>17:25 - 17:50</b></p>	<p><b>Davor J. Korcok</b> <i>Abela Pharm d.o.o., Serbia</i></p>	<p><b>Biophotons and their application in pharmacy</b></p>
<p><b>17:50 - 18:15</b></p>	<p><b>M. Arturo Lopez-Quintela</b> <i>iMATUS, University of Santiago de Compostela, Spain</i></p>	<p><b>Wet-chemical synthesis and catalytic properties of metal clusters of small atomicity without protecting ligands</b></p>

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# Parallel Session

## Day 1

## Room 2

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**Day 1 - Room 2 - Raffaello B**

**08:00 - 09:00 Onsite Registration & Seating Arrangement**

**09:00 - 09:30 Introduction & Open Ceremony**

**Session 1 - Raffaello B**

**Keynote Presentations (Duration: 1hr)**

**09:30 - 10:00** **Yuri Grin**  
*Max-Planck-Institut für  
Chemische Physik fester Stoffe,  
Germany* **Catalysis on Intermetallic Compounds:  
Perspectives and Challenges**

**10:00 - 10:30** **Ge Wang**  
*University of Science and  
Technology Beijing, China* **Element Doping Strategy for  
Highly Efficient Catalyst**

**10:30 - 10:55 (Refreshment & Coffee - Duration: 25min)**

**Session 2 - Raffaello B**

**Oral Presentations (Duration: 2hr 05min)**

**10:55 - 11:20** **Giulia Mazzocanti**  
*Sapienza University of Rome,  
Italy* **Synthesis of copper-functionalized  
amide-linked covalent organic framework  
and its application as a heterogeneous  
catalyst in click reactions**

**11:20 - 11:45** **Matthieu RIVALLIN**  
*Université de Montpellier,  
France* **Treatment of biorefractory organic  
pollutants in water with titanium suboxide  
reactive electrochemical membranes**

**11:45 - 12:10** **Ravishankar G. Kadam**  
*CATRIN-RCPTM, Palacky  
University, Czech Republic* **Intermetallic Copper-Based Electride  
Catalyst with High Activity for C-H Oxidation  
and Cycloaddition of CO<sub>2</sub>**

**12:10 - 12:35** **Beata Tryba**  
*West Pomeranian University of  
Technology in Szczecin, Poland* **Thermo-photocatalytic  
decomposition of VOCs on TiO<sub>2</sub>**

**12:35 - 13:00** **Karolina Kietbasa**  
*West Pomeranian University of  
Technology in Szczecin, Poland* **From nonporous carbon spheres derived  
from molasses through mesoporous spheres  
to microporous carbons for CO<sub>2</sub> adsorption**

**Memorable Group Photo & Selfie**

**13:00 - 14:00 (Tempting Buffet Lunch - Duration: 1hr)**

### Session 3 - Raffaello B

#### Oral Presentation Cont.. (Duration: 2hr, 05min)

14:00 - 14:25	<b>Philippe Pierrat</b> <i>University of Lorraine, CNRS, France</i>	<b>From Biomass Wastes toward Luminescent Graphene Quantum Dots</b>
14:25 - 14:50	<b>Ianasi Catalin</b> <i>Coriolan Dragulescu" Institute of Chemistry, Romania</i>	<b>New materials based on bismuth carbonate with directed properties for precious metals recovery</b>
14:50 - 15:15	<b>Jiri Rathousky</b> <i>J. Heyrovsky Institute of Physical Chemistry, Czech Republic</i>	<b>Smart materials for the environmentally friendly cleaning and protection of cultural heritage artifacts</b>
15:15 - 15:40	<b>Miguel Rocha</b> <i>CeNTI – Centre for Nanotechnology and Smart Materials, Portugal</i>	<b>Solutions for medication monitoring through the application of flexible electronics and smart materials</b>

#### Poster Presentation (Duration: 25min)

15:40 - 16:05	<b>Eliska Mikyskova</b> <i>J. Heyrovsky Institute of Physical Chemistry, Czech Republic</i>	<b>The effect of high air flow velocity on the photocatalytic degradation of Nox</b>
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#### 16:05 - 16:25 (Refreshment & Coffee - Duration: 20min)

### Session 4 - Raffaello B

#### Oral Presentation Cont.. (Duration: 1hr 15min)

16:25 - 16:50	<b>Jongwook Park</b> <i>Kyung Hee University, South Korea</i>	<b>Three-color white electroluminescence utilizing perovskite quantum dots and organic emitters</b>
16:50 - 17:15	<b>Sarah Bogas</b> <i>CeNTI – Centre for Nanotechnology and Smart Materials, Portugal</i>	<b>Printed electronics for pharmaceutical and food packaging</b>
17:15 - 17:40	<b>Tomasz Panczyk</b> <i>Jerzy Haber Institute of Catalysis and Surface Chemistry, Poland</i>	<b>A Smart Carrier of Carmustine Anticancer Drug. Properties And Mechanism of Action Predicted by Molecular Simulations</b>



<b>17:40 - 18:05</b>	<p><b>Samane Maroufi</b>  <i>University of New South Wales, Australia</i></p>	<p><b>Synthesis of Flexible Mn<sub>1-x-y</sub>(CexLay)O<sub>2-δ</sub> Ultrathin-Film from end-of-life Ni-MH batteries</b></p>
<b>18:05 - 18:30</b>	<p><b>Dheeraj Kumar</b>  <i>Indian Institute of Technology Delhi, India</i></p>	<p><b>Top-down synthesis of nonpolar graphene quantum dots</b></p>
<b>18:30 - 18:55</b>	<p><b>Sweety Rani</b>  <i>Indian Institute of Technology, Delhi, India</i></p>	<p><b>3D printed value-added products from polypropylene waste</b></p>
<p><b>*** End of Day 1 ***</b></p>		

## Day 2 - Room 1 - Raffaello A

**08:30 - 09:00** Introduction & Open Ceremony

### Session 1 - Raffaello A

#### Keynote Presentations (Duration: 1hr)

**09:00 - 09:30** **Antonio Monopoli**  
*University of Bari Aldo Moro, Italy* **Pd-catalyzed oxidative homo-coupling of alkenes for the conjugated diene synthesis in ionic liquids**

**09:30 - 10:00** **Antonia Iazzetti**  
*University of the Sacred Heart, Italy* **Advances in transition metal-assisted synthesis and functionalization of heterocycles**

**10:00 - 10:20 (Refreshment & Coffee - Duration: 20min)**

#### Keynote Presentations Cont.. (Duration: 1hr 30min)

**10:20 - 10:50** **Lucia Steenkamp**  
*CSIR, Chemicals Cluster, South Africa* **Industrial Biocatalysis in South Africa**

**10:50 - 11:20** **Laura Scrano**  
*University of Basilicata, Italy* **Innovative methods for the recycling and reuse of contaminated water: the Nanowat project**

**11:20 - 11:50** **Yongdan Li**  
*Aalto University, Finland* **Challenges and progresses of large-scale electric energy storage with flow electrochemical reactors**

### Session 2 - Raffaello A

#### Oral Presentations (Duration: 1hr 40min)

**11:50 - 12:15** **Qianyuan Qiu**  
*Aalto University, Finland* **Fast oxygen reduction and evolution kinetics enabled by  $\text{LaNi}_{0.5}\text{Co}_{0.5}\text{O}_3$  perovskite cathode for a molten salt  $\text{Li-O}_2$  battery**

**12:15 - 12:40** **Patricia Concepcion**  
*Instituto de Tecnologia Quimica (CSIC-UPV), Spain* **Rational design of catalysts for efficient  $\text{CO}_2$  activation**

12:40 - 13:05	<b>Ewelina Kusiak-Nejman</b> <i>West Pomeranian University of Technology in Szczecin, Poland</i>	<b>Carbon spheres modified with APTES (aminosilane) for CO<sub>2</sub> capture</b>
13:05 - 13:30	<b>Carlo Boaretti</b> <i>University of Padova, Italy</i>	<b>Performance improvement of electrospun membranes for water treatment by coupling AOPs with composite catalytic systems</b>
<b>Memorable Group Photo &amp; Selfie</b>		
<b>13:30 - 14:15 (Tempting Buffet Lunch - Duration: 45min)</b>		
<b>Session 3 - Raffaello A</b>		
<b>Oral Presentations Cont.. (Duration: 2hr 05min)</b>		
14:15 - 14:40	<b>Michael G. Organ</b> <i>University of Ottawa Canada</i>	<b>Designing Purpose-Built Ligands for Catalysts: "Say Live and Let Die...."</b>
14:40 - 15:05	<b>Timo Repo</b> <i>University of Helsinki, Finland</i>	<b>The use of co<sub>2</sub> as a building block</b>
15:05 - 15:30	<b>Maria Giorgia Cutrufello</b> <i>Università di Cagliari, Italy</i>	<b>Direct biogas methanation on Ni/CeO<sub>2</sub> catalysts obtained from soft-templated mixed oxides</b>
15:30 - 15:55	<b>Ilaria Longobardo</b> <i>Heraeus Precious Metals, Germany</i>	<b>Platinum Catalysts for the Lignin Conversion into Phenolics as Bio-based Resource for Phenolic Resins</b>
15:55 - 16:20	<b>Matthias Eisenacher</b> <i>TH Köln University of Applied Sciences, Germany</i>	<b>Re-treated zeolites for the HOCK rearrangement in the cumene process</b>
<b>16:20 - 16:40 (Refreshment &amp; Coffee - Duration: 20min)</b>		
<b>Session 4 - Raffaello A</b>		
<b>Poster Presentations (Duration: 50 min)</b>		

16:40 - 17:30	<p><b>Hyun-Ji Kim</b>  <i>Institute for Advanced Engineering, South Korea</i></p>	<p><b>Demonstration of syngas production process directly using low-concentration CO<sub>2</sub> from process exhaust gas</b></p>
	<p><b>Yeji Lee</b>  <i>Kyungpook National University, South Korea</i></p>	<p><b>A study on dry reforming reaction on Ni-based catalyst for direct utilization of exhaust gas</b></p>
	<p><b>José Fenoll</b>  <i>Murcia Institute of Agricultural and Environmental Research and Development, Spain</i></p>	<p><b>Biological-photocatalytic (TiO<sub>2</sub>/Na<sub>2</sub>S<sub>2</sub>O<sub>8</sub>/solar) coupled pilot plant for wastewater detoxification (pharmaceuticals and pesticides) and its reuse for tomato crop irrigation</b></p>
	<p><b>Weishuo Li</b>  <i>University of Oxford, UK</i></p>	<p><b>Chemiresistive polymer percolation network gas sensor created with a nanosphere template</b></p>
17:30 - 18:00 <b>Poster Evaluation &amp; Best Poster Awards (Duration: 30min)</b>		
<b>Group Photo &amp; End of Conference</b>		

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**Parallel Session**

**Day 2**

**Room 2**

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## Day 2 - Room 2 - Raffaello B

09:00 - 09:30 **Introduction & Open Ceremony**

### Session 1 - Raffaello B

#### Keynote Presentations (Duration: 1hr)

09:30 - 10:00 **Guillard Chantal**  
*Université de Lyon, France* **Can the photocatalytic process contribute to our energy and environmental concerns?**

10:00 - 10:30 **Giuseppe Bonura**  
*CNR-ITAE, Italy* **Direct hydrogenation of CO<sub>2</sub> into DME: catalytic and technological aspects**

10:30 - 10:50 (Refreshment & Coffee - Duration: 20min)

#### Keynote Presentations Cont.. (Duration: 1hr 30min)

10:50 - 11:20 **Julien Vieillard**  
*Normandy University, France* **Surface modification of lignocellulosic material for adsorption and photocatalysis**

11:20 - 11:50 **Piotr Cyganowski**  
*Wroclaw University of Science and Technology, Poland* **The powerful response for the major environmental threats. The catalytic hydrogenation of aromatic nitro compounds over rhenium-based nanocatalysts**

11:50 - 12:20 **Frank Gupton**  
*Virginia Commonwealth University, USA* **Novel Carbon Support Systems for Palladium Catalyzed Cross Coupling Reactions**

### Session 2 - Raffaello B

#### Oral Presentations (Duration: 50min)

12:20 - 12:45 **Vivien DALIGAUX**  
*Université de Toulouse, France* **Regeneration of coked catalysts used in plastics pyrolysis: ozonation as an alternative process to oxygen oxidation**

12:45 - 13:10 **Anna Srebowata**  
*Polish Academy of Sciences, Poland* **Catalytic continuous-flow hydrogenation processes for the formation of vitamin and drugs precursors**

#### Memorable Group Photo & Selfie

13:10 - 14:00 (Tempting Buffet Lunch - Duration: 50min)

#### Oral Presentation Cont.. (Duration: 2hr 05min)

14:00 - 14:25 **Lucia Tonucci**  
*Università degli Studi "G. d'Annunzio" di Chieti-Pescara, Italy* **Metal nanoparticles in the hydrogenation reactions in water**

<b>14:25 - 14:50</b>	<b>Francesca Coccia</b> <i>Università degli Studi "G. d'Annunzio" di Chieti-Pescara, Italy</i>	<b>Pd and Rh supported on ovine wool for catalytic reductions in batch and in flow mode</b>
<b>14:50 - 15:15</b>	<b>Amos Bardea</b> <i>Holon Institute of Technology (HIT), Israel</i>	<b>Producing Portable Microreactors into Closed Volume</b>
<b>15:15 - 15:40</b>	<b>Dehhaoui Salma</b> <i>IbnTofail University, Morocco</i>	<b>Characterization and application of hybrid synthesized by sol-gel method</b>
<b>15:40 - 16:05</b>	<b>Rida El-bardai</b> <i>IbnTofail University, Morocco</i>	<b>Development of a novel glasses based on phosphate and its application as a promising adsorbent for crystal violet dye removal</b>

**16:05 - 16:30 (Refreshment & Coffee - Duration: 25min)**

**Session 3 - Raffaello B**

**Poster Presentation Cont.. (Duration: 1hr)**

<b>16:30 - 17:30</b>	<b>Lourenço Bastos</b> <i>University of Minho, Portugal</i>	<b>Numerical simulations to support the development of magnetized gears</b>
	<b>Cátia Araújo</b> <i>University of Minho, Portugal</i>	<b>Dielectric/Electronic ink study for electronic circuit combination</b>
	<b>Sónia Miranda</b> <i>University of Minho, Portugal</i>	<b>An experimental study of the effect on mechanical properties of virgin and recycled high- density Polyethylene blends</b>
	<b>Diana Dias</b> <i>University of Minho, Portugal</i>	<b>A study on carbon vs silver inks conductivity resistance in In- Mould Electronics (IME) process</b>
	<b>Rita Marques</b> <i>University of Minho, Portugal</i>	<b>Powder Injection Molding simulation to study the influence of flow behaviour of highly filled materials with magnetic particles for automotive application</b>

**17:30 - 18:00 Poster Evaluation & Best Poster Awards (Duration: 30min)**

**Group Photo & End of Conference**

**\*\*\* End of Day 2 & Conference \*\*\***



4<sup>th</sup> Global Summit on

# CATALYSIS & CHEMICAL ENGINEERING

April 13-14, 2023 | Rome, Italy

# Keynote Forum

## Day 1

(Room-1)

CHEMICAL CATALYST 2023





4<sup>th</sup> Global Summit on

# CATALYSIS & CHEMICAL ENGINEERING

April 13-14, 2023 | Rome, Italy

## Sharmila M. Mukhopadhyay

Frontier Institute for Research in Sensor Materials  
(FIRST), University of Maine Orono, ME 04469, USA

### Hierarchical Biomimetic Nanocatalyst Architectures

This talk will focus on hierarchical hybrid nanocatalyst architectures that mimic natural biological surfaces like microvilli and dendrites, where a larger substrate is bonded to progressively smaller functional entities to provide high levels of solid-fluid interaction in compact space. The main challenge of fabricating such hybrid solids is to create durable primary bonds between individual components having different size, shape and composition. Recent advances in defect engineering and deposition techniques have enabled our team to fabricate such catalysts, which combine the surface advantages of nanomaterials with the robustness of larger membranes.

A variety of pure and core-shell nanoparticles have been anchored on carpet-like arrays of electrically and thermally conducting carbon nanotubes (CNT) covalently bonded to porous carbon scaffolds. The nanotube carpets create 1000-10,000X increase

in nanoparticle attachment sites without any significant change in weight or volume, and prevent the nanocatalysts from coalescing. Materials characterization is performed using scanning & transmission electron microscopy, X-Ray Diffraction and X-Ray Photoelectron Spectroscopy techniques. Silver particles have shown anti-microbial properties and palladium-based nanocatalysts have shown degradation of halogenated contaminants in water. This talk will focus on halogenated compounds such as carbon tetrachloride, trichloroethylene, triclosan, and atrazine. Degradation rates and pathways investigated using HPLC, LC-MS and GC-MS studies complete step-wise chlorine removal in all cases in the presence of hydrogen. Moreover, the same material could be reused for multiple cycles in flowing liquid. These studies clearly show that this type of catalyst architecture can provide sustainable and eco-friendly clean water technologies.

#### BIOGRAPHY

Dr. Sharmila Mukhopadhyay is Director of the Frontier Institute of Research in Sensor Technologies (FIRST) and Professor of Mechanical Engineering at University of Maine. Her recent research involves multifunctional nanomaterials and surface engineering strategies for energy, environment, and biomedical applications. She received B.S. and M.S. degrees from Indian Institute of Technology and Ph.D. from Cornell University. Prior to joining FIRST, she was Professor of Mechanical and Materials Engineering at Wright State University (WSU) and founding Director of their National Academies-Grand Challenges Scholar's Program, as well as Center for Nanoscale Multifunctional Materials. She is an elected Fellow of the American Ceramic Society, and past Jefferson Science Fellow with the National Academies, where she was Senior Scientific Advisor for the US Department of State.

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## Hugo de Lasa

Chemical Reactor Engineering Centre (CREC), University of Western Ontario, London, Ontario, Canada, N6A 5B9

### The CREC Fluidized Riser Simulator a Unique Tool for Catalytic Process Development

The CREC Riser Simulator is a mini-fluidized bench scale unit invented and implemented in 1992, at the CREC (Chemical Reactor Engineering Centre), University of Western Ontario. The CREC Riser Simulator can be operated at short reaction times, in the 3 s to 20 s range. The present presentation describes and evaluates the original basic concept of the 1992-CREC Riser Simulator Unit, and the improved design of the 2019-CREC Riser Simulator. Both the initial and the enhanced units are specially engineered to allow the rigorous assessment of both catalyst performance and catalytic reaction kinetics. Kinetic parameters of relatively simple and accurate mathematical models can be calculated using experimental data from the CREC Riser Simulator. Since its inception

in 1992, the CREC Riser Simulator has been licensed to and manufactured for a significant number of universities and companies around the world. Several examples of scenarios where the CREC Riser Simulator can be employed to develop fluidized bed catalytic and heterogeneous reactor simulations are reported in this review. Among others, they include (a) hydrocarbon catalytic cracking, (b) the catalytic conversion of tar derived biomass chemical species, (c) steam and dry catalytic methane reforming, (d) the catalytic oxydehydrogenation of light paraffins, (e) the catalytic desulfurization of gasoline, and (f) biomass derived syngas combustion via chemical looping. In this review, special emphasis is given to the application of the CREC Riser Simulator.

#### BIOGRAPHY

Dr. de Lasa is a professor at the Department of Chemical and Biochemical Engineering, University of Western Ontario. He graduated in 1971, with a "Cum Laude" Doctoral degree from the Université de Nancy, in France. Prof. de Lasa is the author of more than 400-peer reviewed publications, 1 book, and 12 U.S. and Canadian patents, as well as the editor of 6 book chapters. He is an innovative teacher who has been actively involved training 56 PhD and 41 MEdSc theses. He is the founding director of the UWO-Chemical Reactor Engineering Centre (CREC). Since its inception in 1987, CREC has received significant financial support, and has been collaborating with industries and governmental agencies from about 25 countries. [https://www.eng.uwo.ca/chemical/faculty/delasa\\_h/](https://www.eng.uwo.ca/chemical/faculty/delasa_h/).

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## Alessia Ciogli

Department of Chemistry and Drugs Technologies,  
Sapienza University of Rome, Italy

### Multifaceted use of mass spectrometry in catalysis: from selection of organocatalyst to the investigation of reaction mechanism and related intermediates

**E**lectrospray ionization mass spectrometry (ESI-MS) is an ideal method to go insight the catalyzed reactions due to its ability to gently transfer ionic species or ionized forms of neutral species in the condensed phase into the gas phase. In particular, its tandem version ESI-MS/MS and, more recently, the IR multiple-photon dissociation (IRMPD) spectroscopy are now established as important tools to study reaction mechanisms in solution and to characterize intermediates. This communication presents, in the first part, the off-line ESI-MS reaction monitoring experiments applied in catalytic processes mediate by well-known chiral primary amines (1,2-diaminocyclohexane, 1,2-diphenylethylenediamine, 9-amino-9-deoxy-9-epiquinine). The approach allow for an alternative

screening of reaction conditions, for a better understanding of reaction mechanism and for obtaining preliminary results about reaction rate. In addition, if combined with enantioselective HPLC analysis, the methodology could be useful in the selection of the catalytic system which induce higher stereoselectivity. In the second part, an example of structural elucidation of reaction intermediates was presented. Reaction models starting from readily available indolyl-methyl-acetates and N soft nucleophiles has been investigated by ESI-MS and IRMPD spectroscopy analyses suggesting the key role of highly reactive 2-alkylideneindolenines and 3-alkylideneindoleninium in the functionalization of carbinol precursors.

#### BIOGRAPHY

Assistant Professor in Organic Chemistry, Dep. of Studies and Technologies of Drug, Sapienza University of Rome.

**RESEARCH ACTIVITY:** The main interests were addressed on i) synthesis of chiral stationary phases for enantiomeric separations, ii) study of molecular recognition processes by HPLC, iii) stereochemical investigation of chiral molecules, specially of stereolabile species through dynamic HPLC and NMR experiments and, more recently, iv) development of supported organocatalysts for asymmetric reactions in heterogeneous systems. These studies are the result of an "interdisciplinary nature" research that affects both the synthetic organic chemistry, the stereochemistry, the chemical of materials and the separation science.

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## Püntener Kurt

Department of Process Chemistry & Catalysis, Synthetic Molecules Technical Development, F. Hoffmann-La Roche Ltd, Grenzacherstrasse 124, CH-4070 Basel, Switzerland

### Highlights & New Insights in Asymmetric Hydrogenation of Keto (Enol) Esters

The presentation gives an insight into the role of the Catalysis & Flow Reactions unit at F. Hoffmann-La Roche Ltd in the development of new drugs, particularly in transition metal catalyzed asymmetric hydrogenations of C=O and C=C bonds. Recent highlights such as

a) Ru-catalyzed hydrogenation of methyl 3-oxotetradecanoate affording (R)-3-hydroxy-tetradecanoate as first chiral intermediate in a 2nd generation process of Roche's anti-obesity drug Xenical, and

b) Ir-catalyzed hydrogenation of keto enol esters affording chiral triols which serve as key building blocks for drug candidates to treat inflammation diseases

will be presented. Particularly, results will be reported of our quantum mechanical investigation of the asymmetric hydrogenation of  $\beta$ -ketoesters catalyzed by  $[\text{RuCl}_2((\text{R})\text{-MeOBIPHEP})(\text{MeOH})_2]$ ,

which is generated in situ from  $[\text{Ru}(\text{OAc})_2((\text{R})\text{-MeOBIPHEP})]$  (1) and HCl. Thereby, HCl not only acts as an activator for the catalyst as it has a dramatic effect on the reaction itself: While  $\text{HCl} / 1 = 2$  leads to rather poor results (36% ee and 13% conv. after 4 h at  $\text{S} / \text{C} = 50'000$ ),  $\text{HCl} / 1 = 20$  results in high efficiency (>99.9% conv.) and enantioselectivity (>99% ee favoring the opposite enantiomer) under other-wise identical conditions. It will be outlined, that a highly selective HCl pathway becomes operational under acidic conditions, which outcompetes moderately selective pathways dominating under neutral conditions. In the 2nd part of the lecture, a dual Ir catalyst systems will be presented which offers a cost-attractive alternative to the previously employed Ir-SpiroPAP single catalyst system in the asymmetric hydrogenation of a set of keto enol esters delivering chiral triols with high diastereo- and enantioselectivity.

#### BIOGRAPHY

I was born on August 7<sup>th</sup>, 1965 in Schattdorf (CH), where I received my primary and secondary schooling. After senior high school I studied Chemistry at the ETH Zürich where I carried out my undergraduate work in the group of Prof. D. Seebach.

Following my diploma work in 1990, I conducted my Ph. D. research under the supervision of Prof. P. S. Pregosin, at the inorganic department at the ETH Zürich on the synthesis of optically active tridentate nitrogen ligands and their application in Pd(II) catalyzed aldol reactions.

From 1994 to 1995, I was post-doctoral fellow in the research groups of Prof. L. S. Hegedus (Colorado State University, Fort Collins USA) where I prepared biologically relevant tetraazamacrocycles via chromium carbene chemistry

1996, I spend a 6 month post-doc in the research groups of Prof. P. Knochel (Phillips University Marburg / Germany), where I synthesized new chiral phosphine and amine ligands for transition metal catalyzed asymmetric (transfer-) hydrogenations.

In 1996, I started industrial work at F. Hoffmann-La Roche Ltd in Basel (CH) in the catalysis group at Process Research & Synthesis. Main activities included the identification and scale-up of transition metal catalyzed reactions and enabling catalyst supply via in-house preparation or collaborations with major catalyst suppliers

In 2011, I was promoted to Group Leader at Process Research & Synthesis and 2013 to Head Process Research at preclinical CMC. In the later role, I was responsible to lead 5 lab teams in preclinical process research activities for small molecule, peptide and oligonucleotide projects to ensure the timely hand over of robust, cost-efficient and scalable processes to allow for API supplies for tox and clinical phase 1 studies.

Since 2019, I am heading the Catalysis & Flow Reactions unit at Synthetic Molecules Technical Development. This unit targets to create and develop sustainable metal and enzyme catalyzed transformations as well as syntheses in flow mode to support Roche's pipeline project most effectively.

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4<sup>th</sup> Global Summit on  
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## A highly efficient and sustainable route for nitro benzene reduction with Copper Nanoparticles and Glycerol

**Katia Martina, Maria Jesus Moran Plata and Giancarlo Cravotto**

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The search for sustainable alternatives for use in chemical synthesis and catalysis has found an ally in non-conventional energy sources and widely available green solvents. In the last decade, copper heterogeneous catalysis gained more and more attention. Being part of important building blocks in organic synthesis, the selective reduction of aromatic nitro compounds represent fundamental procedures in organic synthesis. Many synthetic routes have been described for both reactions via the catalytic hydrogenation with reducing agents such as H<sub>2</sub>, NaBH<sub>4</sub>, formic acid or hydrazine hydrate and different homogeneous and heterogeneous metal catalysts.

Herein we report an efficient synthesis of copper nanoparticles (CuNPs) and their application in efficient hydride-free reduction of aromatic nitro compounds. Experimental studies provide support for a reaction pathway in which the Cu(0) NPs catalysed transfer hydrogenation of nitrobenzene to aniline proceeds via the condensation route and high chemoselectivity toward aniline or azobenzene could be achieved varying the nature of the hydrogen donor source. Enabling technologies, such as microwave and ultrasound irradiation are shown to enhance heat and mass transfer, whether used alone or in combination, resulting in a decrease in reaction time from hours to minutes.

### Biography

Katia Martina is Associate professor of Organic Chemistry at the University of Torino (Italy). Her research interests are in the area of green organic synthesis, preparation of new solid supported organometallic catalysts, benign solvents or solvent free reaction conditions and derivatization of carbon based nanomaterials. Her studies focus on innovative synthetic procedures carried out under non-conventional techniques: microwave-assisted chemistry, Sonochemistry, flow chemistry and mechanochemistry. 78 scientific papers, 4 book chapters and 9 patents and several communications to scientific meetings document her research.

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## Rhodium-Centered Stereogenic Complex with a Tripodal Tetradentate Ligand

**Ricardo Rodríguez**

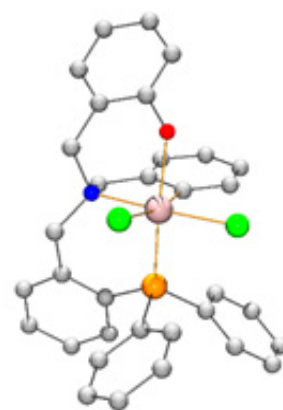
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Chiral complexes are an essential tool as chiral catalysts in asymmetric synthesis. Usually, chiral transition metal catalysts locate their chiral motif on the ligands, in the vicinity of the metal center thus inducing chirality in catalytic processes to a greater or lesser extent. In a complementary way, we [1] and others, [2] are exploring during the last few years how chiral transition metal complexes with stereogenic metal centers are able to transfer chiral information to catalytic products with high efficiency. These complexes are synthesized employing only achiral ligands, the metal center being the unique chiral motif. The successful application of this type of metal complexes to a wide variety of catalytic processes has led to a considerable expansion of the asymmetric catalysis toolbox.

In this work, we describe the completely diastereoselective synthesis of the chiral complexes  $[\text{RhCl}_2(\kappa^4\text{-L})]$  (1) and  $[\text{Rh}(\kappa^4\text{-L-H})(\text{NCMe})_2][\text{SbF}_6]$  (2) containing a new tripodal tetradentate ligand. The resolution of the racemic mixture of 2 has been achieved through

kinetic resolution using enantiopure (S)-2-(4-isopropyl-4,5-dihydrooxazol-2-yl)phenol as a chiral auxiliary. The results of catalytic tests on the 1,3-dipolar cycloaddition reaction proving that the chirality is efficiently transferred from the metal to the substrate.

1. Carmona, M., Rodríguez, R., Passarelli, V., Lahoz, F. J., García-Orduña, P., Carmona, D. *J. Am. Chem. Soc.* 2018, 140, 912–915.
2. Zhang, L., Meggers, E. *Acc. Chem. Res.* 2017, 50, 320–330.



*X-ray structure of 1*

### Biography

Ricardo Rodríguez studied chemistry at the University of Zaragoza (Spain) and received his Ph.D. degree in inorganic chemistry from the University of Zaragoza. After postdoctoral research at the Fundamental and Applied Heterochemistry Laboratory-LHFA (Toulouse, France), he started working as a Tenure Track in the Department of Inorganic Chemistry at Chemical Synthesis and Homogeneous Catalysis Institute-ISQCH (Zaragoza, Spain). Since 2021, he has been a Staff Scientist at the Spanish National Research Council-CSIC (Spain). His research is in the fields of metal-centered stereochemistry and transition metal frustrated Lewis pairs for catalysis.

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## Polyethyleneimine-based materials: novel heterogeneous catalysts for sustainable organic transformations

**Alessandro Sacchetti, Laura Riva, Gloria Nicastro and Carlo Punta**

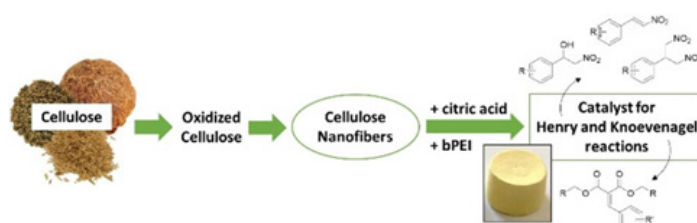
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Polyethyleneimine (PEI), thanks to the presence of nitrogen atoms, is known to be a suitable material for catalysis. In most cases, PEI is used as a grafting agent or as a support for catalytically active metal species whereas only few cases report its use in amine-catalyzed organic transformations. In our team, we developed a new class of cellulose-PEI-based materials obtained by the combination of TEMPO-oxidized cellulose nanofibers (TOCNF) with branched polyethyleneimine (bPEI) and citric acid (CA). The result is a nano-porous material with the characteristics of a Cellulose-based Nano-Sponge (CNS) to be used as catalyst for organic reactions. In this contest, the preparation of heterogenous catalysts from biomass sources is of great interest: beside the use of cellulose from renewable sources, the possibility to employ raw materials and waste as a source has been also explored, thus moving forward to reducing environmental impacts of organic transformations. Herein we report on the use of PEI based CNSs as heterogenous catalyst

for organic reactions, with particular attention to the synthesis of precursors of interest for the pharmaceutical industry. In a first work [1], the CNSs have been used as basic amine catalyst for the Henry and Knoevenagel reactions, affording the products in good yields and selectivity.

Then, exploiting the coordinating capability of PEI, the material has been loaded with metals, namely copper, zinc and palladium. These new catalysts proved to be very effective in metal catalyzed organic reactions as acetal formation [2] and Suzuki-Miyaura coupling between aryl halides and phenyl boronic acid in water.

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2. Riva, L.; Lotito, A. D.; Punta, C.; Sacchetti, Gels 2022, 8, 54.



### Biography

Alessandro Sacchetti graduated in Chemistry in 1998 and got a PhD in Chemical Science in 2002 at the university of Milan. Since 2008 is associate professor of the department of Chemistry, Material and Chemical engineering "G. Natta" at Politecnico di Milano. Research interests are in the field of the synthesis of organic molecules as biological active compounds and heterocyclic ligands for metal catalysis. More recently he become interested in the chemical modification of polymer for the production of biomaterials for drug release and of functional materials for heterogenous catalysis. He also has a strong collaboration with many chemical companies for the development of new products and procedures in the view of technology transfer. He is coauthor of more than 110 peer reviewed publications.

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## Sustainable electrocatalytic processes using iron phosphide thin films

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Electrocatalysis using low-cost materials is a promising, economical strategy for remediation of water contaminated with inorganic contaminants, organic chemicals and microorganisms. Here, we report the use of iron phosphide (Fe<sub>2</sub>P, FeP) for electrocatalytic reduction of nitrate ion (NO<sub>3</sub>), degradation of rhodamine B (RhB) dye; and inactivation of Escherichia coli (E. coli) bacteria. The electrochemical reduction reaction of the nitrate ion (NO<sub>3</sub>), a widespread water pollutant, to valuable ammonia (NH<sub>3</sub>) is a promising approach for environmental remediation and green energy conservation. Particularly, FeP and Fe<sub>2</sub>P phases were successfully demonstrated as efficient catalysts for NH<sub>3</sub> generation. Detection of the in-situ formed product was achieved using electrooxidation of NH<sub>3</sub> to nitrogen (N<sub>2</sub>) on a Pt electrode. The Fe<sub>2</sub>P catalyst exhibits

the highest Faradaic efficiency (96%) for NH<sub>3</sub> generation with a yield (0.25 mmol h<sup>-1</sup> cm<sup>-2</sup> or 2.10 mg h<sup>-1</sup> cm<sup>-2</sup>) at -0.55V vs. reversible hydrogen electrode (RHE). Using a thin film of Fe<sub>2</sub>P precatalyst, we also conducted degradation of RhB dye (achieved 98% efficiency) and inactivation of E. coli (100%). Under an applied bias of 2.0 V vs. reversible hydrogen electrode in the presence of in situ generated reactive chlorine species it was found efficient oxidation of organics and dyes. Recycling test revealed that Fe<sub>2</sub>P precatalyst exhibits excellent activity and reproducibility during degradation of RhB. High-performance liquid chromatography with UV-Vis detection further confirmed the electrocatalytic (EC) degradation of the RhB dye. These findings suggest that Fe<sub>2</sub>P-iron phosphate electrocatalyst could be an effective water remediation agent.

## Biography

Saim Emin received his PhD (2010) in the field of chemistry from Saitama University, Japan. Later, he joined the Advanced Photovoltaic Center at the National Institute for Materials Science, Japan. In 2012 Dr. Emin was awarded with a Marie-Curie Career Integration Grant funded by the European Commission. Since 2019 he holds a position as Associate Professor of Chemistry at the University of Nova Gorica, Slovenia. He has been a chair in many conferences including at the conference series "International Conference on Functional Nanomaterials and Nanodevices". Dr. Emin has co-authored more than 40 publications in peer-reviewed international journals and has given talks at more than 25 international conferences`.

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## Engineering copper nanoparticle electrodes for tunable electrochemical reduction of carbon dioxide

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The electrochemical conversion of CO<sub>2</sub> into high values molecules such as carbon monoxide (CO), methane (CH<sub>4</sub>) and ethylene (C<sub>2</sub>H<sub>4</sub>) represent an intriguing strategy to store the unutilized renewable electricity while simultaneously addressing the issue of global warming. All the three abovementioned molecules can be obtained by conducting CO<sub>2</sub> electrolysis catalyzed by copper (Cu)-based catalysts. In this work, gas diffusion electrodes fabricated with different Cu nanoparticles are engineered in order to properly tune the selectivity toward one of these reaction products. In particular, for low catalyst loading (0.25 mg cm<sup>-2</sup>), the CH<sub>4</sub> production is favored, while the selectivity shifts toward C<sub>2</sub>H<sub>4</sub> for intermediate (1.0 mg cm<sup>-2</sup>) loadings. Eventually, for larger

values (3.0 mg cm<sup>-2</sup>) the CO production becomes the most relevant. In particular, a 46% peak selectivity for C<sub>2</sub>H<sub>4</sub> has been obtained on 1.0 mg cm<sup>-2</sup> loaded electrode at a current density of 600 mA cm<sup>-2</sup>. The C<sub>2</sub> products including C<sub>2</sub>H<sub>4</sub>, ethanol and acetate reach 50-60% selectivity at high reaction rates ( $\geq 600$  mA cm<sup>-2</sup>) and relatively low cell voltages ( $\leq 4.0$  V). Both bulk and local CO generation rates, and charge transfer mechanism dominated by capacitive effects are found to be responsible for the observed variations in the selectivity while changing the Cu nanoparticle loading. The present work provides a new strategy for steering the CO<sub>2</sub> reduction reaction selectivity by simple electrode engineering beyond material development.

### Biography

Dr. Zeng is currently an assistant professor in Politecnico di Torino, and mainly works on applied electrochemistry in different research fields like fuel cells, Li-O<sub>2</sub> batteries and CO<sub>2</sub> electrolyzers. She has (co)authored 38 papers in international journals with high impacts and two patents. She was awarded Premio di Dottorato 2013 "Fondazione De Nora" by Società Chimica Italiana. She has great passion in training young researchers, and has been tutoring numerous master and Ph.D students in materials Science and Technology, Chemical Engineering, Nanotechnology and Physics. She is a Guest Associate Editor, Topic Editor and Topical Advisory Panel Member for various journals, and active as a Reviewer for many prestigious journals like ACS Catalysis, ACS.

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## Electrocatalysis on carbide and graphene-based materials for electrochemical devices

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Hydrogen is considered an energy vector for the transition towards a future based on the use of renewable energy. In this context, electrolyzers (EL) allow to obtain H<sub>2</sub> of high purity, which would be a great advantage when used in low-temperature fuel cells (PEMFC). However, the development of these systems and their entry into the market are conditioned, in part, by the use of noble metal catalysts (platinum group metals, PGMs). This communication presents the latest results of our research group in the preparation of materials free of noble metals with high activity for the reactions on the electrodes of these devices.

In the field of EL, transition metal carbides appear as an alternative to PGMs showing good catalytic activity towards the electrochemical generation of hydrogen. In the search for

cheaper materials, the use of ionic liquids that improve the mechanical resistance and electrical conductivity of the resulting composite materials has also been proposed. The study of the hydrogen evolution reaction by means of differential electrochemical mass spectrometry (DEMS) has allowed us to delve into the mechanistic aspects of this process.

On the other hand, graphene materials (MGs) have recently shown their potential as a support for electrocatalysts, with important activities, even similar, to those of materials based on platinum and other noble metals. The doping of MGs also appears as an appropriate method to modify and control the electrochemical response in reactions such as oxygen electroreduction (in PEMFC) or the evolution of hydrogen and oxygen (in EL).

### Biography

Dr. Elena Pastor is professor at the University of La Laguna (ULL) and principal investigator of the Surface Science and Electrocatalysis Group. Her research activity has focused on the development of materials for electrochemical energy conversion devices, such as electrolyzers, fuel cells and batteries. She has published more than 180 articles in international journals and presented around 300 communications in congresses. Her research work has been recognized by her institution with the ULL 2018 Research Award. She has been Director of the ULL Institute of Materials and Nanotechnology in 2010 and 2011 and President of the Ibero-American Electrochemical Society between 2016 and 2018. Since 2019 she is Vice Dean of the degree in Chemistry at the ULL.

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## Phase-transfer catalysts for sustainable stereoselective synthesis of amino acid and lactone derivatives

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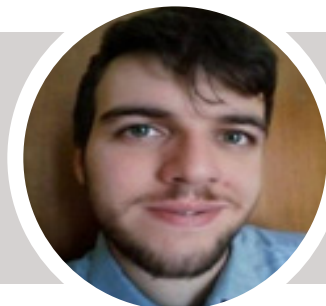
Phase-transfer catalysis (PTC) is a well-established technique widely applied in organic synthesis both on laboratory and industrial scale, which combines the advantages of mild, simple and inexpensive procedures with reduced environmental impact. One of its most relevant aspects is the possibility to carry out base-promoted reactions of weakly acidic substrates avoiding the use of water sensitive reagents and strictly anhydrous conditions, with obvious benefits in terms of process safety, reduced costs and energy saving. In the light of this, we focused our recent studies in developing PTC processes aimed to the stereoselective synthesis of potentially bioactive molecules, by

making use of both widely employed and newly designed catalysts. This oral presentation gives an extensive overview of these achievements, describing the application of novel chiral macrocyclic catalysts to the synthesis of amino acid derived compounds as well as the use of privileged quaternary ammonium salt catalysts for the preparation of trifluoromethylthio-amino acid derivatives. Furthermore, the development of new stereoselective C–C bond formation reactions of unsaturated lactones, such as  $\gamma$ -butenolides and isobenzofuranones, has provided a convenient strategy for the synthesis of bioactive natural products and drugs containing the phthalide and the phthalan core.

### Biography

Giorgio Della Sala received his Ph.D. in chemistry from the University of Salerno in 2002. He worked as a visiting scientist in the labs of Dr. Susagna Ricart at the Department of Molecular Materials of Materials Science Institute of Barcelona (CSIC), in 2003, and of Prof. Karl Anker Jørgensen at the Center for Catalysis, University of Aarhus, in 2007. He held the position of Assistant Professor at the Department of Chemistry and Biology "A. Zambelli", DCB) during 2004-2020. Since December 2020, he is Associate Professor at DCB, University of Salerno. His research is mainly focused on the development of stereoselective metal- and organo-catalyzed methodologies and their application to the synthesis of natural products and potentially bioactive analogs.

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## Gold (I)-catalyzed an efficient and mild synthesis of 3,8- Diarylidene-2,7-dioxaspiro[4.4]nonane-1,6-diones

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**3**,8-dibenzyl-2,7-dioxaspiro[4.4]nonane-1,6-diones are a class of compounds widespread in natural and bioactive compounds. For instance, natural compounds isolated from *Carpesium abrotanoides* with a similar  $\gamma$ -dilactones scaffold, such as dicarabrol A, dicarabrone C, and dipulchellin A, demonstrated promising biological activities such as anti-inflammatory, antitumor, antiplasmodial, and bactericidal effects.

For their remarkable properties, these compounds have always drawn the attention of researchers, and their construction by means of alternative routes is still a challenging research area. Herein, we reported on the synthesis of spiro lactones

starting from substituted dialkynylmalonic acids. In particular, we demonstrated that functionalized symmetric or unsymmetric biarylacetylenic malonic acids may be efficiently cyclized under mild conditions in the presence of JohnPhosAu(MeCN)SbF<sub>6</sub>. The reaction's scope was evaluated via the preparation of different substituted dialkynylmalonic acids that in the reaction condition gave the corresponding  $\gamma$ -arylmethylene-spirobis lactones in excellent yields (96–100%). The results of our investigation show that this process may represent an easy and efficient approach to highly valuable building blocks of natural products or biologically active compounds.

### Biography

Dario Allevi was born in Como in 1992. He obtained his master's degree in Medicinal Chemistry and Technology at the University of Pavia in 2018, discussing an experimental thesis about chemoenzymatic synthesis. After graduation he worked as a R&D technician in Goglio S.p.A., Como, for two years (2018–2019). In October 2019 he moved to Politecnico di Milano as a research fellow in enzymatic organo-catalysis. After, in 2021, he turned his attention into the preparation of modified graphene to tune his suspensibility in various solvents. He started his PhD in 2022 at University of the Sacred Heart, Rome, where he actually works.

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## Effect of lithium co-doping on structural, morphological and photocatalytic properties of RE-doped ZnO

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<sup>3</sup>Universidad Complutense de Madrid, Spain

**Nanostructured ZnO:** RE particles doped with Li were prepared by the polyol method at low temperature and short growth times. Different lithium contents were evaluated, keeping the atomic% of RE constant. The samples were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), BET, XPS, Raman and photoluminescence. X-ray diffraction patterns have shown that the samples have a polycrystalline wurtzite structure. No secondary phases have been identified in the concentrations studied. The Cell parameter has been determined, and the crystallite size of Scherrer's formula has been calculated considering the three

most important diffraction peaks. Transmission electron microscopy (TEM) indicated the purity of the phase obtained and its high crystallinity. Raman analysis confirms the hexagonal structure of wurtzite ZnO. Morphological and size changes have been observed by SEM and TEM, particularly from hemispherical NPs (ZnO NPs) to spindle-shaped particles (ZnO codoped with Li-Nd). The photocatalytic behavior of the Li-RE codoped ZnO NPs has been evaluated. The highest photocatalytic activity was obtained after 45 min with a 100% degradation of a aqueous solution of Rodhamine B (2.5 ppm).

### Biography

Professor ME Rabanal has 23 years of research experience. She joined the Carlos III University of Madrid to complete her Doctoral Thesis. Her research career is linked to the synthesis, optimization, and characterization of functional ceramic nanomaterials by "bottom-up" methods. Currently she focuses its research on: the improvement of the photocatalytic properties of pure oxidic semiconductors or doped with transition metals by different methods: Spray pyrolysis, hydrothermal method, polyol, co-precipitation, ..., and the synthesis, optimization, and characterization of "up-converting" luminescent materials co-doped with rare earth elements.

Dr. Rabanal has 78 articles in the Web of Science. Her research lines have led to important relationships with international research centres (ITS SASA-Belgrade, BUAP\_Mexico, RWTH Aachen University, UAC-Mexico, ...), national research centres (IMDEA-Nanociencia, IMDEA-Materiales, CENIM, Instituto de Geociencias (UCM-CSIC, ...), and companies with research activities (Nanoair solution, Cegasa, ...). She has supervised more than 23 final degree and master's degree projects. He has directed 7 Doctoral Theses and is directing 1 in progress.

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## Structural and morphological evaluation of Gd-Li co-doped ZnO system with improved photocatalytic activity

**Adalyz Ferreiro Fernández<sup>1</sup>, A. Urbieto<sup>2</sup>, P. Fernández<sup>2</sup>,  
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Semiconductor materials, especially rare-earth elements doped ZnO, have attracted great interest for their advanced properties and potential applications, for example, in the photocatalytic degradation of emergent pollutants. These materials are becoming necessary for decreasing environmental effects in the water of antibiotics, hormones, drugs, toxic organic dyes, and organic compounds. In this research work, Gd, Li codoped ZnO nanoparticles were synthesized by an easy, cheap, and friendly process; the polyol method. Keeping constant the Gd atomic %, different Li dopant content has been evaluated. Many experimental techniques, such as X-ray diffraction (XRD), scanning electron microscopy (SEM), Transmission electron microscopy (TEM), BET: Brunauer–Emmett–Teller analysis (BET),

photoluminescence (PL), Raman Spectroscopy, X-ray Electron Spectroscopy (XPS) have been used. X-ray diffraction patterns have shown that all samples present a wurtzite structure. No secondary crystalline phases have been identified. The reticular parameters and the crystallite size by Scherrer's Formula have been calculated. By FESEM and HRTEM, morphological and size changes have been observed. X-ray Electron Spectroscopy (XPS) and  $\mu$ -Raman Spectroscopy analysis indicate the incorporation of the dopant into the structure. Rhodamine B as a model pollutant has been used for photocatalytic performance, and the kinetic study has been carried out using Langmuir- Hinshelwood model.

**Key words:** nanoparticles, doped zinc oxide, photocatalytic degradation, Rhodamine B.

### Biography

Bachelor's Degree in Chemistry from University of Havana, Cuba (2012) and a Master's Degree in Materials Science and Engineering from University of Carlos III of Madrid, Spain (2019), Her experience with polymeric materials, nanoparticles and composites for bone tissue restoration, controlled drug release and general biomedical applications through different preparation methods and characterization techniques, she has working as a researcher and laboratory analyst at Center for the Mining Metallurgical Industry (CIPIMM) basically in the Atomic Absorption Spectrometry (AAS) and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) techniques. Currently, she is a PhD candidate in Materials Science & Engineering at UC3M and teaching assistant, her research focuses on synthesis and structural, morphological and functional characterization of nanoparticles of ZnO doped with rare earths and alkaline elements by polyol method for wastewater treatment and environmental applications, moreover of evaluation of photocatalytic activity and antibacterial properties of hybrid semiconductor oxides on emerging pollutants in wastewater.

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## Synthesis of propiolic acids by silver-catalyzed insertion of CO<sub>2</sub> to terminal alkynes

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During the last decades, the enormous consumption of fossil fuels, related to industrialization and therefore to the increasing consumption of energy, has produced the emission of large volumes of carbon dioxide (CO<sub>2</sub>) in the atmosphere, causing worrying climate change. In this scenario, all countries have focused their attention on reducing CO<sub>2</sub> emissions or using it as a reagent, for the synthesis of molecules with higher added value. The development of catalytic strategies for the use of carbon dioxide is one of the most interesting objectives of sustainable chemistry. CO<sub>2</sub> can be a C1 feedstock for the synthesis of value-added products, but it is a thermodynamically and kinetically stable molecule, which makes it difficult to use as a reactant. Among the various transformations

developed in recent years (e.g., cyclic addition of CO<sub>2</sub> to epoxides, hydrogenation of formic acids, etc.), the carboxylation of the terminal alkyne, catalyzed by transition metal complexes, is one of the most useful. Silver and copper salts can activate the carbon dioxide molecule in presence of a base in mild reaction conditions. Stabilized by N-heterocyclic carbene silver complexes (NHC-Ag) have shown interesting activity in the insertion of carbon dioxide to terminal alkynes by C-H activation.

Here, we report the synthesis and the characterization of new silver complexes, stabilized by NHC ligands, asymmetrically substituted on nitrogen atoms, and having different groups on the backbone of heterocycle and their catalytic activity in the reaction of carboxylation of terminal alkynes.

### Biography

Marco Sirignano was born in Pordenone (Italy) in 1992 and studied chemistry at the University of Salerno (BSc 2015 and MSc 2018). He completed his Ph.D. in 2022 under the supervision of Professor Pasquale Longo. During his research activity, he worked on the synthesis of silver and gold complexes stabilized by carbenes N-heterocyclic and their study in A<sub>3</sub> coupling reactions and in the hydroamination of terminal and internal alkynes. He published several papers with interesting results in collaboration with other research groups.

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## Formate Dehydrogenases Mimics as Catalysts for Carbon Dioxide Reduction

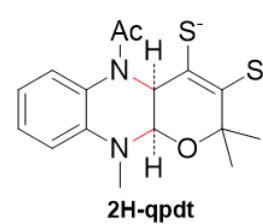
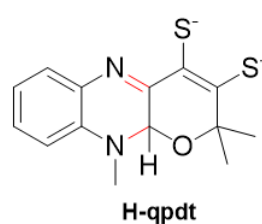
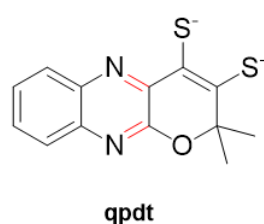
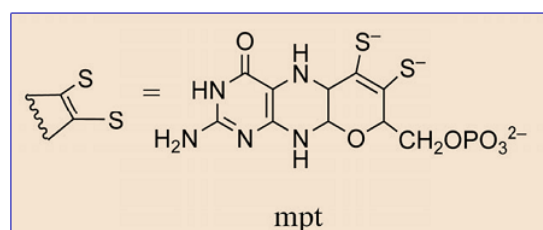
**Yun L, Thibault Fogeron, Jean-Philippe Porcher and Marc Fontecave**

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**C**O<sub>2</sub>/HCOOH interconversion is a biological reaction catalyzed by formate dehydrogenases (FDHs) whose active site might serve as a source of inspiration in order to design new molecular catalysts for CO<sub>2</sub> conversion to formic acid. FDH has Mo/W mononuclear centers in which the metal ion is chelated by two identical dithiolene ligands, called molybdopterin (mpt). The natural complex found in FDHs has never been isolated due to fast decomposition. Synthetically mimicking such active sites is highly challenging.

In order to study complexes relevant to FDH,

we have prepared three original dithiolene ligands, namely qpdt, H-qpdt and 2H-qpdt. The major difference between three ligands resides in the oxidation state of the central pyrazine ring which displays a high degree of similarity with mpt. The corresponding Mo-oxo complexes were synthesized and structurally characterized. The ability of these complexes to perform H<sup>+</sup>/CO<sub>2</sub> reduction in both electrochemical and photochemical conditions has been addressed. For the first time, a Mo-dithiolene complex is found active as a catalyst for the photoreduction of CO<sub>2</sub> into HCOOH and CO.



### Biography

Yun Li was born in Shanghai, China where she graduated in Pharmaceutical Chemistry at the East China University of Science and Technology. She obtained her PhD degree in Organic Chemistry in Paris at the Pierre et Marie Curie (Paris 6) University. She moved to Geneva (Switzerland) and Columbus (Ohio, USA) as a post-doctoral fellow working Medicinal Chemistry. She is a permanent researcher of the French National Center for Scientific Research (CNRS) at the Collège de France / Paris Sorbonne University. Her research interests are focused on the design and synthesis of biomimetic complexes for diverse applications. Currently, she works on bioinspired Molybdenum-dithiolene complexes as homogeneous catalyst for proton/carbon dioxide reduction.

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## Biophotons and their application in pharmacy

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Biophotons are light particles which every cell emits in order to communicate with other cells. Biophotons create a system that could be responsible for chemical reactions within cells, cellular communication through the organism and overall regulation of the biological system, including embryonic development. Each cell emits its own characteristic light pattern. Biophotonic medicine or food supplement uses any type of substrate (aqueous solutions, capsules, tablets, powders etc.) electromagnetically charged with biophotons that regulate energy homeostasis and thus biochemical homeostasis. In order to use biophotons of substances for practical purposes, these signals must be stored in a computer and must be perfectly identical to the original ones. We have measured a specific

energy emitted by the finished products with vitamins and minerals in the form of tablets, stored it electronically and used it to all finished products with vitamins and minerals in order to increase their efficacy. Furthermore, we have performed research and measured the quantity of vitamin C in urine in a sample of people which used during the 30 days a product without the application of photonic activation and after their photonization. Tablets which were previously photonized have presented slightly higher quantities of vitamin C content in urine after 30 days, because light energy activated vitamin C molecules. In the future, further research will be performed in order to completely evaluate their bioavailability in healthy individuals and individuals with impaired physiological functions

### Biography

Davor J. Korčok, PhD, specialist of Industrial Pharmacy and specialist of Food Technology, is the lead auditor in international organization standards for Quality Management Systems. He holds prestigious ECA certificate and has been appointed as internal and external consultant of the Agency for medicinal products and medical devices of Bosnia and Herzegovina, and as the visiting and accredited lecturer at the Faculty of Pharmacy, University of Sarajevo and Belgrade, and for the Health Council of Serbia. Also, he is renowned as a first author and co-author of many scientific researches all published in distinctive scientific magazines, he was an editor of scientific guidelines: "Secrets of intestinal microbiota, modern recommendation for use of probiotic products", published in 2017. He is a member of the board of directors of United Association of Serbia for Quality. In January 2019 he was elected to be president of the Scientific Technical Committee for Pharmacy. Also, he is Assistant professor at the pharmaceutical faculty in Novi Sad. On the position of the General Manager of Abela Pharm, he has been since April 1<sup>st</sup>, 2012.

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## Wet-chemical synthesis and catalytic properties of metal clusters of small atomicity without protecting ligands

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<sup>1</sup>*iMATUS, University of Santiago de Compostela, 15782-Santiago de Compostela, Spain*

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**M**etal nanoclusters show very different properties than both, nanoparticles and bulk, due to the quantum confinement of the free electrons [1]. Such nanoclusters can be seen as super-atoms (or molecules) in which atoms are linked by strong covalent bonds [2]. In the past decade, we have developed wet-synthetic methods, based on kinetic control [5] without binding ligands, to produce monodisperse nanoclusters of small atomicity ( $< \approx 20$  atoms). Such clusters show very unusual catalytic properties. For example, Au<sub>5</sub> clusters display high catalytic activities for the aerobic oxidation of thiophenol to disulphide [3]. Very recently, we have also reported exceptional catalytic activities of Ag<sub>5</sub> clusters for the irreversible aerobic oxidation of thiols [4], increasing the catalytic activity in the series  $O_2 < H_2O_2 < OH$  radicals, which was used to demonstrate a new catalytic approach to cancer therapy [4]. We have also reported that

such clusters can be used as catalytic radical scavengers in industrially relevant processes involving detrimental free radical formation such as polymer stabilization [5].

In this talk we will describe the synthesis of nanoclusters by kinetic control and revise some of their catalytic properties.

1. See e.g. Protected Metal Clusters: From Fundamentals to Applications, Tatsuya Tsukuda, Hannu Häkkinen, Elsevier, Amsterdam, 2015.
2. see e.g. P. Jena, Q. Sun, Chem. Rev. Am. Chem. Soc. 118 (2018) 5755–5870.
3. A. Corma et al. Nat. Chem. 5 (2013) 775–781.
4. V. Porto et al. Adv. Funct. Mater. (2022) 2113028.
5. I.R. Arias et al. J. Colloid Interface Sci. 628 (2022) 437–447.

### Biography

Full Professor of Physical Chemistry at the University of Santiago de Compostela (USC, Spain). Postdoc in Germany at MPI für Biophysikalische Chemie, Göttingen and University of Bielefeld. Visiting Professor at MPI für Metallforschung, Stuttgart, Germany; Centre for Magnetic Recording Research, UCLA, USA; Yokohama Natl. University, Japan and Research Centre for Materials Science, Nagoya, Japan. Solvay Award in Chemistry and Burdinola Award in the Field of New Nanotechnologies in Chemistry. Co-founder and Principal Scientific Advisor of the company NANOGAP ([www.nanogap.es](http://www.nanogap.es)), founded in 2006 and dedicated to the production of nanomaterials and metal clusters. In 2019 co-founder of Arjuna Therapeutics ([www.arjunatherapeutics.com](http://www.arjunatherapeutics.com)) to explore metal clusters as a new class of treatment to address major problems in oncology. Since 2005 Co-editor of the Journal of Colloid and Interface Science. He has published more than 350 publications (h-index 59), is co-author of 26 licensed, international patents. His current research interests are: synthesis and properties of nanomaterials and “ligand-free” metal clusters by soft chemical techniques; synthesis of anisotropic nanomaterials and nanocomposites; and applications of metal clusters in catalysis, electrocatalysis, photocatalysis, and study of their therapeutic properties.

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4<sup>th</sup> Global Summit on  
**CATALYSIS &  
CHEMICAL  
ENGINEERING**

April 13-14, 2023 | Rome, Italy

**Keynote Forum**

**Day 1**

(Room-2)

**CHEMICAL CATALYST 2023**



## Yuri Grin

Max-Planck-Institut für Chemische  
Physik fester Stoffe, Dresden, Germany

### Catalysis on Intermetallic Compounds: Perspectives and Challenges

Intermetallic compounds attract a lot of attention in catalysis community during the last decades. This family of inorganic substances introduces an alternative and very powerful way to develop new materials for heterogeneous catalysis and electrocatalysis. The variety of crystal structures, the unique atomic interaction between the atoms and – as a consequence - an ability to tailor the electronic state of atoms are consolidated basis for the application of intermetallic compounds in catalysis. Important recent developments in the quantum chemistry in position space, especially in the analysis of chemical bonding using the electron-localizability approach, make the quantitative description of the surface state and estimation of the adsorption energies of certain adsorbates possible, allowing the interpretation

of the experimentally obtained catalytic results. However, such scenario is visible only in case of catalysis under reductive conditions, allowing to preserve the inherent features of intermetallic compounds. In case of oxidative environment, intermetallic compounds undergo changes in bulk or surface region and catalytic performance depends on the actual state of the surface under dynamic conditions of catalytic process. In this case, insight into chemical bonding is a way to shed a light on the chemical behavior of the intermetallic compound in reaction media. This scenario will be illustrated with intermetallic compounds, which were studied catalysts for hydrogenation reaction, and as electrocatalysts for oxygen evolution reaction.

#### BIOGRAPHY

Yuri Grin is director at the Max-Planck-Institut für Chemische Physik fester Stoffe in Dresden, head of the department Chemical Metals Science. His research topics are experimental and theoretical investigations on chemistry and physics of intermetallic compounds. In particular chemical bonding in intermetallic compounds, and their catalytic and thermoelectric properties are in focus of studies.

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## Ge Wang

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### Element Doping Strategy for Highly Efficient Catalyst

Photocatalytic water splitting into hydrogen is convincing as an intriguing route for transform solar-light energy to chemical energy. Metal chalcogenide semiconductors exhibit favorable photocatalytic H<sub>2</sub> production property due to the strong visible-light response ability and appropriate energy band structure. Especially, chalcogenide semiconductors with unique 2D ultrathin structure can effectively shorten the diffusion distance and promote the photogenerated. However, the potential wells of chalcogenide semiconductors block the photoexcited electrons traveling along Z axis, and then result in low charges separation and transport efficiency. Recently, our group a series of efficient catalyst by element doping strategy. For example, Ni, In co-doped ZnIn<sub>2</sub>S<sub>4</sub> photocatalyst was

prepared by a microwave-assisted solvothermal method. The rapid crystallization of ZnIn<sub>2</sub>S<sub>4</sub> resulted in partial In atoms substituted Zn atom during the formation of [ZnS]<sub>4</sub> layer. In doping in tetrahedral Zn sites increases the electron delocalization around In sites, hence reduces the electronic potential wells along Z axis. Ni doping in tetrahedral Zn sites decreases the negative charge on the S sites, which balances the H adsorption/desorption, further boosting the photocatalytic activity. As a result, Ni, In co-doped ZnIn<sub>2</sub>S<sub>4</sub> possess an optimal photocatalytic H<sub>2</sub> evolution property. These works afford an available inspiration on promoting the photoexcited charges separation/transport and balancing H absorption/desorption by controllable doping tactics to signally boost the photocatalytic performance.

#### BIOGRAPHY

Ge Wang received her Ph.D. in Chemistry from the Michigan Technological University in 2002. Currently she is a professor and Ph.D. supervisor in the School of Material Science and Engineering at the University of Science and Technology Beijing. In 2012, she became a special chair professor endowed by the Chang Jiang Scholars Program of the Ministry of Education. Her research interests focus on creating complex materials structures with nanoscale precision using chemical approaches, and studying their functionalities including catalytic, energy storage and energy saving properties etc.

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# CITY ATTRACTION OF ROME





4<sup>th</sup> Global Summit on

# CATALYSIS & CHEMICAL ENGINEERING

April 13-14, 2023 | Rome, Italy

## Scientific Sessions

### Day 1

(Room-2)

CHEMICAL CATALYST 2023



## Synthesis of copper-functionalized amide-linked covalent organic framework and its application as a heterogeneous catalyst in click reactions

**Giulia Mazzocanti, Maria Aurora Guarducci and Alessia Ciogli**

*Department of Chemistry and Drugs Technologies, Sapienza University of Rome, Italy*

Covalent Organic Frameworks (COFs), first studied in 2005 by Yaghi et al., are a class of organic crystalline polymers with permanent porosity and a highly ordered structure, consisting of light elements (i.e., C, N, O and B). They show excellent chemical stability in organic solvents and can withstand harsh, acidic, and basic conditions. Unlike other polymers, a significant feature of COFs is that they are structurally predesignated, synthetically controllable, and functionally manageable. In this work, an amide-linked COF has been synthesised via the solvothermal method using

pyridine-2,6-dicarboxylic, activated by thionyl chloride, and tetrakis(4-aminophenyl)methane (TAPM) as building blocks. Such structure enables strong coordination with metals, that can be loaded on COF. In this contribution, we focus on coordination with copper that occurs by wet impregnation with a solution of copper acetate. The copper-loaded COF (Cu@COF) (3% w/w) was obtained and successfully used, after a reduction step with a solution of ascorbic acid, as a heterogeneous catalyst for the alkyne-azide click reactions, obtaining higher yields than the analogous reaction in the homogeneous phase.

### Biography

Assistant Professor in Organic Chemistry, Dep. of Studies and Technologies of Drug, Sapienza University of Rome.

#### RESEARCH ACTIVITY

Giulia Mazzocanti obtained her PhD from the Sapienza University of Rome in 2018 with a thesis regarding advanced techniques in separation science for unravelling the complexity of natural substances from small chiral molecules to large proteins. Her research activity concerns i) the synthesis of chiral and achiral stationary phases, ii) various strategies to drastically reduce harmful and difficult-to-dispose organic solvents in chromatography, iii) and to make some synthetic processes more sustainable through heterogeneous catalysis.

In 2021, she became Assistant Professor at her Alma Mater.

Co-Author of 25 publications in international journals. H index = 9(Scopus font).

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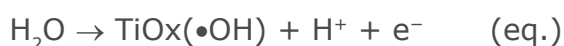
## Treatment of biorefractory organic pollutants in water with titanium suboxide reactive electrochemical membranes

**Matthieu Rivallin<sup>a</sup>, Charlotte Lebesgue<sup>a</sup>, Flavien Turin<sup>b</sup>,  
Chaïma Gomri<sup>a</sup>, Eddy Petit<sup>a</sup>, Sophie Cerneaux<sup>a</sup>, Mona Semsarilar<sup>a</sup>,  
Yoan Pechaud<sup>b</sup>, Clément Trelu<sup>b</sup> and Marc Cretin<sup>a</sup>**

<sup>a</sup>Institut Européen des Membranes, IEM, UMR 5635, Univ Montpellier, CNRS, ENSCM, Montpellier, France

<sup>b</sup>Université Gustave Eiffel, Laboratoire Géomatériaux et Environnement, EA 4508, UPEM, 77454 Marne-la-Vallée, France

The development of compact and robust water treatment technologies plays an important role both environmentally and economically. In this perspective, this work is based on the development of titanium suboxide anodic materials and their integration in advanced oxidation electrochemical membrane processes allowing the treatment of wastewater with biorefractory micropollutants. It constitutes a real challenge for the development of an effective technology that can be adapted to any other organic pollution. The proposed approach involves the implementation of the oxidation of water on a porous ceramic anode to generate hydroxyl radicals (eq.), very reactive and non-selective species to lead to almost total mineralization (transformation into CO<sub>2</sub>, H<sub>2</sub>O and small non-toxic carboxylic acids) of pollutants.



The porosity of the sub-stoichiometric titanium oxide conductive membrane integrated in a pilot coupling membrane filtration and anodic oxidation is the key parameter for improving mass transport of target compounds from the bulk to the electrode surface. We will present here our latest results, obtained for the degradation of organic compounds (paracetamol, carbamazepine, tetracycline and PFAS) in different types of water (pure water or real effluents). Our results showed that pollutants could be mineralized up to 90% in a single pass through the membrane by optimizing feed fluxes and electrolysis currents. The evolution of the treated waters toxicity and the byproducts formation were monitored. The current efficiency for mineralization of organic compounds was determined and the permeate flows controlled with a view to estimating the viability of this technology.

### Biography

Dr. Matthieu RIVALLIN received his PhD in Chemical Engineering and Materials Chemistry from Mines Paris (France) in 2003. He first served, in 2004, as a post-doc at the University "La Sapienza" at Rome (Italy). He then joined, in 2005, the European Membrane Institute of Montpellier with permanent position as associated professor of the National Graduate School of Chemistry of Montpellier (France). His main research areas concern the development of membrane filtration systems coupled with advanced oxidation processes for wastewater treatment. His expertise mainly includes the elaboration of active membranes based on metal oxide and their integration in coupling membrane filtration and advanced oxidation process for removing non-biodegradable organic pollutants from water.

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## Intermetallic Copper-Based Electride Catalyst with High Activity for C-H Oxidation and Cycloaddition of CO<sub>2</sub>

**Ravishankar G. Kadam<sup>1</sup>, Dagmar Zaoralova<sup>1,2</sup>, Miroslav Medved<sup>1</sup>, Priti Sharma<sup>1</sup>, Giorgio Zoppellaro<sup>1</sup>, Michal Otyepka<sup>1,2</sup>, Radek Zbořil<sup>1,2</sup>, Hideo Hosono<sup>3</sup> and Manoj B. Gawande<sup>1,5</sup>**

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<sup>5</sup>Institute of Chemical Technology Mumbai-Marathwada Campus Jalna, Maharashtra 431213, India

Inorganic electrides have been proved to be efficient candidates for incorporating transition metals, which can effectively act as active sites and delivered an outstanding catalytic performance. In this work, a reusable and recyclable copper-based intermetallic electride catalyst (LaCu<sub>0.67</sub>Si<sub>1.33</sub>), in which the Cu sites activated by anionic electrons with low-work function are uniformly dispersed in the lattice framework, shows vast potential for the selective C-H oxidation of industrially important hydrocarbons and cycloaddition of CO<sub>2</sub> with epoxide. This leads to the production of value-added cyclic carbonates under mild reaction conditions.

Importantly, the LaCu<sub>0.67</sub>Si<sub>1.33</sub> catalyst enables much higher turnover frequencies for the C-H oxidation (up to 25 276 h<sup>-1</sup>) and cycloaddition of CO<sub>2</sub> into epoxide (up to 800 000 h<sup>-1</sup>), thus exceeding most non noble as well as noble metal catalysts. Density functional theory investigations have discovered that the LaCu<sub>0.67</sub>Si<sub>1.33</sub> catalyst is involved in the conversion of N-hydroxyphthalimide (NHPI) into the phthalimido-N-oxyl (PINO), which then triggers selective abstraction of an H atom from ethylbenzene for the generation of a radical susceptible to further oxygenation in the presence of O<sub>2</sub>.

### Biography

Dr. Ravishankar G. Kadam studied Chemistry at Institute of Chemical Technology, (Formerly UDCT), Mumbai, India and graduated in 2018 under the supervision of Prof. R.V. Jayaram. He has been awarded with prestigious fellowships such as Senior Research Fellowship (SRF) from (UGC-UPE), University of Mumbai, India during his doctorate degree. He then joined the research group as Postdoctoral fellow with Prof. Radek Zbořil and Prof. Manoj B. Gawande, at Nanocatalysis Laboratory, Czech Advanced Technology and Research Institute (CATRIN- RCPTM), Palacký University Olomouc, Czech Republic. His post-doctoral research includes various areas of chemistry, materials science and catalysis. Specifically, he is actively involved in design of novel heterogeneous and single metal atom catalysts for organic transformations, fine chemical synthesis, electrochemical and energy applications. Currently, he is working as a senior researcher. And he has published 13 research articles in prestigious high impact factor peer reviewed journals.

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## Thermo-photocatalytic decomposition of VOCs on TiO<sub>2</sub>

**Beata Tryba, Piotr Miądlicki and Piotr Rychtowski**

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Photocatalytic decompositions of gaseous acetaldehyde and ethylene were performed on anatase type TiO<sub>2</sub> under UV irradiation at the temperatures of 25-200°C. Acetaldehyde was greatly adsorbed on TiO<sub>2</sub> surface and was partly decomposed via catalytic action of TiO<sub>2</sub> even at room temperature, around 25% of acetaldehyde with inlet gas concentration of around 210 ppm was decomposed, however its mineralization to CO<sub>2</sub> was insignificant. Decomposition of acetaldehyde on TiO<sub>2</sub> increased at higher temperature, however high conversion to the formaldehyde and carbonaceous species was noticed without further mineralization. Generation of CO<sub>2</sub> appeared under UV irradiation. Both, decomposition and mineralization of acetaldehyde on TiO<sub>2</sub> increased under UV irradiation at higher temperature. Although the highest conversion of acetaldehyde (50%) was obtained at 125°C due to the thermo-photocatalysis, abundance of CO<sub>2</sub> formation

was observed at lower temperatures, such as 75-100°C. Ethylene species were poorly reacted with TiO<sub>2</sub> surface under dark conditions, only 5% of ethylene with inlet gas concentration of 50 ppm was decomposed at 300°C. However, under UV irradiation ethylene decomposition was supported through the thermal heating. The highest conversion of ethylene (35%) was observed at the temperature range of 100-150°C. In both cases, thermal assisted photocatalytic process of VOCs decomposition appeared to be advantageous, although acetaldehyde was easier decomposed than ethylene due to its strong interaction with titania surface. Thermal catalysis can enhance the yield of the photocatalytic reactions, but total mineralization of treated VOCs is impossible without UV irradiation.

**Funding:** National Science Centre, Poland, grant nr 2020/39/B/ST8/01514.

### Biography

Prof. Beata Tryba – (2016) Professor at the West Pomeranian University of Technology in Szczecin, Poland. Employed at the Department of Catalytic and Sorbent Materials Engineering; Research topics: photocatalytic materials, environmental technology, materials design and characteristics. Supervisor of 4 doctoral theses and reviewer of 14 ones. (2002) Postdok in Aichi Institute of Technology; (2004) Postdok in Oita University, Japan. (2005) Nominated COST coordinator in Poland, Action 540 "Phonasum". Coordinator of few research projects in Poland financed by Ministry of Science and Higher Education and National Science Centre. Author of around 80 research papers with citations over 2600 and h index =27.

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## From nonporous carbon spheres derived from molasses through mesoporous spheres to microporous carbons for CO<sub>2</sub> adsorption

### Karolina Kielbasa

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Herein, the raw material for preparation of carbonaceous materials was a molasses solution with a sucrose concentration of 1 mol/dm<sup>3</sup>, placed in an autoclave for 12 hours at 200 °C. After hydrothermal synthesis, the sample was removed from the autoclave, rinsed with deionized water until neutral, and dried at 110 °C. After drying, the spherical material obtained from hydrothermal synthesis was activated with solid KOH for 3 hours. The mass ratio of carbon to activating agent (C:KOH) was changed in the range from 1 to 4. The material was heated at 750 °C under nitrogen flow (20 dm<sup>3</sup>/h). The prepared carbon materials containing the decomposition products of potassium hydroxide or potassium carbonate were washed with distilled water to achieve a neutral reaction. Subsequently, the

activated carbon was dried at a temperature of 110 °C for 20 h. The characterization of the activated biocarbon samples was carried out via several instrumental techniques such as XRD, FTIR, Raman, N<sub>2</sub> sorption at the temperature of -196 °C, and CO<sub>2</sub> sorption. The CO<sub>2</sub> adsorption equal to 7.03 mmol/g at the temperature of 0 °C and pressure of 1 bar was achieved. The CO<sub>2</sub> adsorption at 1 bar pressure increases with C:KOH ratio, however at 0.15 bar the trend is reversed. Activation of carbon spheres with potassium hydroxide caused obtaining of carbon materials through mesoporous spheres to microporous carbons. It was found that the specific surface area and total pore volume increase along with an increase in C:KOH ratio, while micropore volume decreases.

### Biography

I received my PhD degree at the West Pomeranian University of Technology in Szczecin at the Faculty of Chemical Technology and Engineering. Currently the Vice-Dean for Student Affairs and Education. I am dedicated to teaching and engaged in the pedagogical transformation for

the education of future chemists and engineers.

Huge fan of Marvel Comics and F1 Racing – of course, Scuderia Ferrari is my favorite team.

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## From Biomass Wastes toward Luminescent Graphene Quantum Dots

**Philippe Pierrat<sup>1</sup>, Pascal Franchetti<sup>2</sup>, Pierre Magri<sup>2</sup> and  
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Graphene quantum dots (GQDs) are new fascinating carbon nanomaterials that are attracting great attention according to their outstanding features in comparison with usual organic dyes and heavy metals-based quantum dots. GQDs display chemical inertness, low photobleaching, low cytotoxicity, excellent biocompatibility, wavelength-tunable luminescence, electronic conductivity and a large surface area. As a consequence, GQDs are useful in many applications such as biosensors, solar cells, electrochemical devices, optical sensors and energy storage devices. However, there was no chemical processes allowing to prepare GQDs in large amount with high yield and low cost to allow the applications to be transferred at the industrial scale. In that context, we recently developed a fast, efficient and reproducible microwave-assisted synthesis of GQDs from various biomass wastes (e.g. oak acorns, date stones, orange peels and

compost) in a straightforward, rapid and high yielding chemical transformation performed under microwave activation allowing preparing GQDs at a large scale. Our procedure affords GQDs with good homogeneity (in terms of size, chemical constitution and photophysical properties) from a wide range of biomass wastes. The soluble particles show excitation-dependent photoluminescence ranging from blue to orange emission wavelength in aqueous solution. Interestingly, dry films of pure GQDs display white light emission under UV excitation, while aggregation-induced quenching is usually observed in the solid state, opening the way toward OLED applications. We further demonstrated the potential of our GQDs as chemical sensors toward various metal traces such as Hg<sup>2+</sup>, Fe<sup>3+</sup> and Sn<sup>2+</sup> with competitive detection limits through a fluorescence quenching mechanism.

### Biography

Philippe Pierrat studied chemistry at the University of Nancy and obtained his Ph.D. in 2006. Next, he joined the research group of Pr. Stefan Bräse for 2 years at the University of Karlsruhe (Germany) with an Alexander von Humboldt post-doctoral fellowship to work on fullerene chemistry. In 2009, he was appointed assistant Professor of Organic chemistry at the University of Strasbourg in the research group of Dr. Luc Lebeau where he was developing therapeutic gene delivery approaches using cationic lipids and carbon nanodots. In 2015, he joined the University of Lorraine as an assistant Professor. His current research interests include the design and synthesis of highly conjugated chemicals such as ullazine derivatives and graphene quantum dots for various applications such as luminescence, sensors and energy (batteries and solar cells).

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## New materials based on bismuth carbonate with directed properties for precious metals recovery

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**M**etals can be the key to a clean environment. So, starting from bismuth carbonate as principal precursor, we developed three series of four samples of bismuth oxide by using the sol-gel method. The process was carried out in an acidic environment. By choosing the sol-gel method, we were able to obtain the final materials at room temperature and thus modify its structure. In order to form better materials polymers and carbons were added in composites. The porosity of the material could be controlled by closely following the requirements of the industry in order to use them in adsorbing precious metals such as gold, silver or palladium. The materials

were characterized by TG, FT-IR, XRD, BET and SEM. The materials indicate a porous structure with the formation of clusters of approximately 10  $\mu\text{m}$  and a specific surface of approximately 40m<sup>2</sup>/g with pores of approximately 10nm.

**ACKNOWLEDGMENT:** This paper was financially supported by the Project "Network of excellence in applied research and innovation for doctoral and postdoctoral programs" / InoHubDoc, project co-funded by the European Social Fund financing agreement no. POCU/993/6/13/153437

We are thankful to the Romanian Academy (Project 4.1.) for the financial support.

### Biography

Dr. Ing. Ianăși Cătălin, Scientific Research III, work at "Coriolan Drăgulescu" Institute of Chemistry, Timisoara, Romania. I have graduated Faculty of Industrial Chemistry and Environmental Engineering, 2007 promotion. As a researcher I have complete the following:

- co-author of 44 scientific articles published in Web of Science-Clarivate Analytics indexed journals; 75 abstracts published in conferences or symposium proceedings; research team member in seven Research Projects; reviewer member at Processes Journal, 275 citations in Web of Science-Clarivate Analytics; Hirsch Index on ISI web of science: 10.

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## Smart materials for the environmentally friendly cleaning and protection of cultural heritage artifacts

### Jiri Rathousky

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Removing unwanted material from the surface of historical artifacts is one of the most important and simultaneously the trickiest operations in restoring cultural heritage. Despite the apparent simplicity, cleaning is a very challenging task for both restorers and scientists/technologists. We have developed a novel patented technology based on a modular principle, combining a microemulsion of environmentally friendly non-ionic surfactants, which is the same for all the substances to be removed from the surface, and specific solvents selected according to the properties of targeted species. The unique features of the developed cleaning systems ensure that their application is highly controlled, selective without affecting the material of the artifact itself, and friendly to the environment and the health of the staff. The method is universal and suitable for various surfaces (stone, glass, metal, or canvas) and substances to be removed (hydrophobic agents,

waxes, oils, polymers, etc.). The developed method was successfully used for the cleaning of materials of Czech historical monuments, such as St. Vitus Cathedral in Prague, or medieval paintings.

Another essential issue in the restoration of historical buildings and stone artifacts is their preventive protection, which not only protects the treated object but also substantially prolongs the necessity of further restoration interventions. We developed a completely new approach to the hydrophobization of surfaces of sandstone and calcareous building materials, based on the formation of a thin hydrophilic layer on a surface of otherwise hydrophobized materials. This unique approach enables the treated materials to retain their natural appearance and properties, which is of major importance for aesthetic reasons and does not limit additional restoration interventions.

### Biography

Jiri Rathousky is the head of the Center for innovations in the field of nanomaterials and nanotechnologies at the J. Heyrovsky Institute of Physical chemistry. His scientific activities represent a fundamental contribution to the development of science on a global scale, both in the field of academic and applied research. They include the discovery of previously unknown phenomena in heterogeneous catalysis and sorption processes and the development of new preparation procedures in the field of nanostructured materials. His work has resulted in the development of novel technologies in the field of environmental engineering and the conservation of our cultural heritage. His Ph.D. students have found significant positions in the field of science both in the Czech Republic and abroad. He fundamentally contributes to the popularization and propagation of science, leading to increased interest among the young generation and the public as a whole.

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## Solutions for medication monitoring through the application of flexible electronics and smart materials

**Miguel Rocha, K. Rodrigues, L. Sousa, J. Pinheiro, C. Oliveira, I. Silva, P. Henriques, G. Ferreira and S. Silva**

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**N**on-adherence to medication is an increasingly recurrent problem, according to data available in the literature, in the United States, 30% to 50% of the adult population does not comply with their prescribed medication. In this context, the development of intelligent solutions capable of interacting with the patient, alerting to the time of taking it, becomes increasingly important. The project "SMART-HEALTH-4-ALL - Smart medical technologies for better health and care" aims to develop innovative solutions for patients, specifically the PPS5 - Medication Management Devices, which aims, through the solution aptAMED, the development of a device that can be attached to the base of any pre-existing medication bottle, giving it new functionalities to assist the user during drug therapy. AptAMED solution includes the combination of flexible sensors, monitoring the drug therapy of the patient. The device includes the development of pressure sensors, including the application

of printed electronics for the development of highly flexible and light devices, which can be easily incorporated in the final solution. On this topic, it were developed both piezoresistive and capacitive sensors, through the combination of conductive inks and functionalized dielectric layers, including a profound study of different dielectric materials. Simultaneously, the developed sensors were optimized in terms of geometry and production processes. Up to this stage, the results obtained demonstrate the capability of these sensors in monitoring weight variations between 500 mg - 100 g. This work was developed in the scope of the SMART-HEALTH-4-ALL project (POCI-01-0247-FEDER-046115; LISBOA-01-0247- FEDER-046115), which is co-financed by Portugal 2020, under the Operational Program for Competitiveness and Internationalization (COMPETE 2020) and Lisbon Regional Operational Programme (LISBOA2020) through the European Regional Development Fund (ERDF).

### Biography

Miguel Rocha holds a master degree in Materials Engineering from the University of Minho. During his academic career, he developed knowledge about the properties and characterization of metallic, ceramic and polymeric materials. Also acquired knowledge in the area of composite materials. In the academic year 2020/2021, he completed a curricular internship at Continental-ITA, in partnership with CeNTI. As part of the internship, he contacted with functional textiles and rubber composites areas, integrating sensing and communication technologies into rubber composites. Since September 2021, Miguel Rocha works as a researcher in the Smart Materials team at CeNTI, being involved in several national and international projects where intelligent materials and solutions are developed.

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## The effect of high air flow velocity on the photocatalytic degradation of NO<sub>x</sub>

**Eliska Mikyskova**

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Nitrogen oxides (NO<sub>x</sub> = NO + NO<sub>2</sub>) are considered as one of the most hazardous pollutant due to their toxicity on human health. Therefore, it is crucial to keep their concentration on the long-term low levels.

Among advanced oxidation processes, heterogeneous photocatalysis is often the only viable route. The effect of relevant process parameters on the efficiency of the photocatalytic technology should be determined. There are four types of these parameters, namely the irradiation, air humidity, the composition of the gaseous mixture and the character of air flow. However, the effect of the character of air flow on the photocatalytic performance was addressed mostly marginally. Up to now, the papers published revealed considerable uncertainties in the flow regime description related to the relatively narrow range of flow parameters, especially the volume rate of flow, velocity or the cross-sectional area.

### Biography

Eliska Mikyskova is the postdoctoral researcher at the Centre for innovations in the field of nanomaterials and nanotechnologies at the J. Heyrovsky Institute of Physical chemistry of the CAS, v. v. i. Her scientific activities include, for example, the remediation of water and air environment using adsorption and photocatalytic processes.

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The present study is aimed at the systematic experimental research into the effect of air flow through the photoreactor at a wide range of conditions, which enables to model realistic situations encountered in the real application of photocatalytic technology for the purification of air. The degradation of NO<sub>x</sub> pollutants (0.1 and 1.0 ppmv) at air flow velocities ranging from 0.02 to 0.7 m s<sup>-1</sup> was tested, the photocatalytic efficiency being determined for various slit heights (5–25 mm) and rate of volume flow (1500–11 000 cm<sup>3</sup> min<sup>-1</sup>). The photocatalysts achieved substantial NO and NO<sub>2</sub> abatement. Pollutant conversion decreased as the air flow velocity increased, with the highest conversion (80%) occurring at 0.1 m s<sup>-1</sup> [1].

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## Three-color white electroluminescence utilizing perovskite quantum dots and organic emitters

### Jongwook Park

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To implement a full-color display in the research field of perovskite or perovskite-structured quantum dots (PeQD), it is necessary to develop a white light emitting device that operates by emitting three primary colors (red, green, and blue). It has emerged as an active research topic. In this study, we report for the first time high-brightness three-color white emission from white-emitting PeQD organic light-emitting diodes (WPeQD-OLEDs) fabricated using PeQD materials and organic emitters. WPeQD-OLED bilayer is prepared by mixing CsPb(Br/I)<sub>3</sub> QDs as a red-emitting PeQD material with N<sup>9</sup>,N<sup>10</sup>-Bis(4-(tert-butyl)phenyl)-N<sup>9</sup>,N<sup>10</sup>-Di-o-Tolylanthracene-9,10-Diamine (p-Tb-o-Me-TAD) used as a green organic emitter. For the blue emission layer, N<sup>1</sup>,N<sup>6</sup>-bis(5-(tert-butyl)-2-methylphenyl)-N<sup>1</sup>,N<sup>6</sup>-bis(2,4-dimethylphenyl)-pyrene-1,6-diamine (3Me-

1Bu-TPPDA), which was used as a blue organic emitter on top of the mixing layer, was deposited through thermal evaporation. A white PeQD-organic light-emitting diode (WPeQD-OLED) with The WPeQD-OLED device was stable during operation and showed emission of three primary colors. In the WPeQD-OLED device, the charge carriers were distributed by the 9-(naphthalen-1-yl)-10-(naphthalen-2-yl)anthracene ( $\alpha,\beta$ -ADN) blue emitting host material, at the molecular orbital level. The electroluminescence (EL) spectrum of the WPeQD-OLED showed EL maxima peaks at 460, 527, and 640 nm. The CIE color coordinates of the emitted light were (0.33, 0.40). The EL results confirmed that the maximum luminance was 49,000 cd m<sup>-2</sup>, the maximum luminance efficiency was 4.48 cd A<sup>-1</sup> and the power efficiency was 2.16 lm W<sup>-1</sup>.

### Biography

Jongwook Park is Professor at Department of Chemical Engineering of Kyung Hee University in Korea. He received his Ph.D. from Korea Advanced Institute of Science and Technology. He is the author of 330 SCI papers and holds 65 patents in the field of organic semiconducting materials. He was chairman of 12 large-scale projects of Korean industry in relation with electronic materials. He received the Prime Minister and President Awards from Korean government in 2012 and 2020. He was also elected SPIE Fellow in 2018 in the United States as well as Kyung Hee University Fellow in 2019.



## Printed electronics for pharmaceutical and food packaging

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Many industries have been implementing strategies to raise awareness among end-users, not only for the proper storage of pharmaceuticals and food supplements, but also to maintain their quality and safety and enhance their shelf-life, even when they are temporarily not stored under ideal conditions. Smart packaging is the best choice for monitoring some parameters that could be responsible for the deterioration of pharmaceuticals and food, and for its protection and preservation.

The SMASUS project aims to develop a passive monitoring solution using printed UV and temperature sensors directly applied to the sleeves of packages in order to monitor and quantify physical parameters that contribute to product quality over time. The developed sensors were flexible and fully printed, produced by screen-printing, a low-cost and useful technique for large- area applications.

The UV sensors were resistive and composed of

metallic oxide-based sensible layers. They were characterized under UV and sunlight conditions, revealing good reproducibility. In the presence of UV and sunlight, the conductivity of the metallic oxide layer increases, demonstrating its efficacy as a UV sensor. To monitor the thermal conditions to which the packages were exposed, printed temperature RTDs (Resistive Temperature Detectors) sensors based on silver ink were developed. The resistance of these sensors showed linear behavior with temperature changes in a range of -20 to 60°C, low hysteresis effect, and good stability over time.

The work was developed in the scope of the "SMASUS - Smart and Sustainable Packaging" project (POCI-01-0247-FEDER-047007; LISBOA-01-0247-FEDER-047007), which was co-financed by

Portugal 2020, under the Operational Program for Competitiveness and Internationalization (COMPETE 2020) through the European Regional Development Fund (ERDF).

### Biography

Sarah Bogas has a master's degree in Biophysics and Bionanosistemas from the physics department of the University of Minho. Since 2020 works as a researcher at CeNTI's Smart Materials department. Her research activities have been focused on the development, integration, and characterization of print electronic systems/sensors. Her work has focused on the production of several printed devices, from heating systems; capacitive and resistive sensors, in different substrates, acquiring knowledge in the development of intelligent textiles and intelligent composites. From the printed devices she also has knowledge and experience in the development of flexible thermoelectric generators. Also possessing knowledge in the study and development of formulations for encapsulants and inks. She has participated in R&D projects, allowing it to acquire skills throughout the process of development, integration, production, and characterization of the R&D product in the industrial process. She has also assumed the role of responsible researcher, leadership, and teamwork skills.

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## A Smart Carrier of Carmustine Anticancer Drug. Properties And Mechanism of Action Predicted by Molecular Simulations

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We found that carmustine (1,3-bis(2-chloroethyl)-1-nitrosourea), BCNU, can be stored in the internal space of carbon nanotube (CNT) for a long time due to hydrophobic interactions. The access of water to carmustine phase in the CNT interior can be controlled by the state of cytosine rich DNA fragments covalently bound to the CNT tips and to the presence of doxorubicin, DOX, molecules intercalated within bundles of DNA fragments. More effective control of water access and subsequent decomposition of carmustine due to the contact with water was observed when some small amount of doxorubicin molecules cork the CNT ends. Our analysis shows that carmustine decomposition products naturally separate when decomposition occurs within the CNT. The alkylating agent, chloroethyl

carbonium cation, spontaneously escapes from the CNT but the carboamoylation agent, chloroethyl isocyanate, is still kept within the nanotube interior. The separation process and release of the alkylating agent needs uncorking the nanotube by doxorubicin molecules. The latter process is likely to occur spontaneously at acidic pH when intercalation of doxorubicin within the DNA fragments becomes ineffective. The features of the proposed molecular model, obtained from molecular dynamics simulations, can be beneficial in design of novel smart drugs carriers to a tumor microenvironment revealing the reduced extracellular pH.

**Acknowledgment:** This work was supported by Polish National Science Centre grant 2017/27/B/ST4/00108.

### Biography

Prof. Tomasz Panczyk studied Chemistry at the Department of Chemistry, Maria Curie-Skłodowska University in Lublin, Poland and graduated in 1997. He then joined the research group of Prof. Władysław Rudziński at the same Department and started his PhD. He received his PhD degree in 2001 at the same institution. Since 2001 he has been employed in Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences in Krakow. Since 2009 he is a Life Member of Clare Hall college in Cambridge, UK. He has published more than 90 research articles in SCI(E) journals.

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## Synthesis of Flexible Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> Ultrathin-Film from end-of-life Ni-MH batteries

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The present work details a three-stage strategy based on selective purification of rare earth oxide (REOs) isolated from end-of-life nickel-metal hydride (Ni-MH) batteries leading to high-yield fabrication of defect-rich Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> film. In step one, major impurities (Fe and Al) were removed from a REE-rich solution. In step two, the resulting solution with trace content of Mn was further purified through electrodeposition which resulted in synthesis of a non-stoichiometric Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> ultra-thin film, with controllable thicknesses (5-650 nm) and transmittance (~29-100%) in which Ce<sup>4+/3+</sup> and La<sup>3+</sup> ions were dissolved in MnO<sub>2-x</sub> lattice. Due to percolation impacts on the optoelectronic properties of ultrathin films, a representative Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> film with 86% transmittance exhibited an outstanding areal capacitance of 3.4 mF•cm<sup>-2</sup>, mainly attributed to the intercalation/de-intercalation of anionic O<sup>2-</sup> charge carriers through the atomic

tunnels of the stratified Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> crystallites. Furthermore, the Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> exhibited excellent capacitance retention of ~90% after 16,000 cycles. Such stability was shown to be associated with intervalence charge transfers occurring among interstitial Ce/La cations and Mn oxidation states within the Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> structure. The energy and power densities of the transparent flexible Mn<sub>1-x-y</sub>(Ce<sub>x</sub>La<sub>y</sub>)O<sub>2-δ</sub> full-cell pseudocapacitor device, with a solid-state electrolyte, was measured to be 0.088 μWh.cm<sup>-2</sup> and 843 μW.cm<sup>-2</sup>, respectively. These values showed insignificant changes under vigorous twisting and bending to 45-180° confirming these materials are intriguing alternatives for size-sensitive energy storage devices. In step three, the remaining solution purified further that led to formation of REOs (La, Ce, and Nd) nanospheres with ~40-50 nm diameter.

### Biography

I hold both a Bachelor and Master's Degree in Chemical Engineering and a PhD in Materials Science and Engineering from UNSW, Australia. I finished my PhD in 2015, now as lecturer I work at School of Materials Science and Engineering, UNSW. In the past 7 years after finishing my PhD, I have taken a variety of topics to work on for the purpose of continuing my research pathway plus working on industrial projects. My research spaces across the fields of high temperature pyrometallurgical processing, sustainability of materials process (waste recycling and materials transformation) and synthesising nano-structure materials from waste for energy storage devices.

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## Top-down synthesis of nonpolar graphene quantum dots

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Polymers are used in many different areas because of their exceptional mechanical and chemical capabilities. In contrast, the globe generates millions of tons of plastic waste every year. Plastic waste has been an issue to a deleterious level over the past decades and needs immediate attention worldwide. The synthesis of high-valued nanomaterials from nonbiodegradable plastic waste has drawn immense attention in recent years. The top-down nanomaterial synthesis approach includes breaking down the larger organic structures at nanoscale using chemical, thermal or mechanical approach. Pyrolysis is one of the mostly preferable techniques used worldwide because of its easy execution and mass scale production possibilities, among all the top-down synthesis approaches. The pyrolysis of plastic

waste in the presence of harsh acidic or basic conditions is the most reported method for the synthesis of different carbon nanoforms. Among all the carbon nanomaterials, zero-dimensional graphene Quantum Dots (GQDs) are considered highly promising because of their extraordinary properties and multidimensional application area. Herein, a microwave-assisted pyrolysis method was developed for the synthesis of nonpolar GQDs from plastic waste in an acid/base free environment. GQDs of single-layered sp<sup>2</sup> structure without any polar functionalities were obtained in size range of less than 10 nm. The inherent nonpolar nature of the GQDs thus obtained unwraps new opportunities of application in various fields including hydrophobic coatings, oil industries, energy sector, and sensors.

### Biography

Mr. Dheeraj Kumar is working in the field of Nanotechnology for past 10 years. He is a final year PhD student in the Department of Textile and Fibre Engineering, Indian Institute of Technology Delhi, India. He has completed M.Sc. (Nanoscience with research) and M.Tech. (Nanotechnology) dual master's degree from Amity Institute of Nanotechnology, Amity University. His expertise includes synthesis of metal, metal oxide and carbon Nanomaterials in polar and nonpolar mediums using various top-down and bottom-up approaches. He has been working in the field of self-cleaning coatings, nano lubricants, energy devices and sensors. He has also founded InstaNANO, a scientific analysis platform used by more than thousands of researchers daily.

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## 3D printed value-added products from polypropylene waste

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The worldwide plastic trash problem has already reached crisis proportions, but the COVID-19 epidemic has exacerbated the need for single-use plastics. It resulted in the unnecessary disposal of plastic, particularly protective gear fabricated from Polypropylene (PP). The pervasiveness of plastic waste has compelled us to seek alternatives to cut down its whopping amount. The porous materials have been widely used in gas separation, support matrix (for catalysts, drugs, etc), water purification and adsorbents, etc. There are many conventional techniques to generate porous monoliths like solvent casting, gas foaming, particulate leaching, and freeze-drying, etc. The emulsion templating method however

offers a viable and convenient technique to produce porous structures with high porosity, interconnectivity and tunability of pores. Therefore, an unexplored water in oil emulsion of PP waste (sack and mask) was developed and utilized as a template to fabricate porous 3D structures. The porous structures depicted mesoporous morphology with a high specific surface area. The samples were found to have a high oil adsorption capacity for gasoline comparable to that of a commercial nonwoven PP absorbent pad. This approach has the potential to be scaled up to make the process commercially viable and can be applied for other plastic wastes as well.

### Biography

Ms. Sweety Rani was born on August 10, 1992 at Faridabad, India. She joined as a PhD Scholar in the Department of Textile and Fibre Engineering, Indian Institute of Technology Delhi, India in July 2019. Prior to joining PhD she has completed M.Sc (Applied Chemistry) degree from Amity Institute of Applied Sciences, Amity University and also worked at Indian Oil Corporation Limited R&D Centre, India for more than a year. She has expertise in synthesis of metal oxide nanocomposites, catalysts, zeolites, emulsion templating, sensors and 3D printing.

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4<sup>th</sup> Global Summit on

# CATALYSIS & CHEMICAL ENGINEERING

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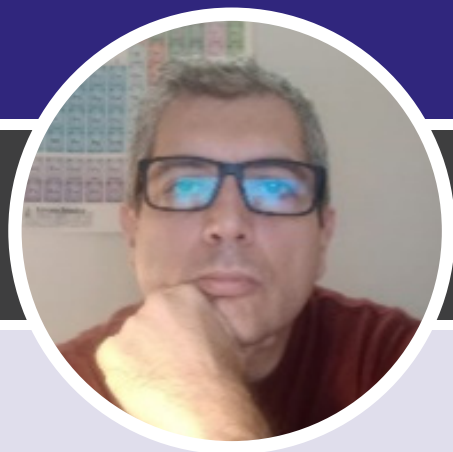
## Keynote Forum

### Day 2

(Room-1)

CHEMICAL CATALYST 2023

## Antonio Monopoli<sup>a,b</sup>

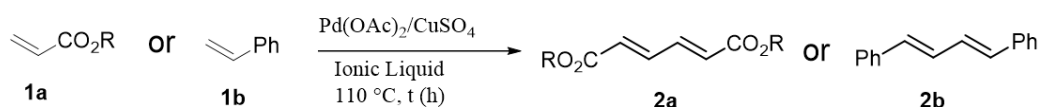


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### Pd-catalyzed oxidative homo-coupling of alkenes for the conjugated diene synthesis in ionic liquids

Conjugated diene fragments are widely distributed in many natural compounds, optical materials, and pharmaceuticals<sup>1</sup>. In particular, 1,4-diarylbuta-1,3-dienes are of substantial importance not only due to their

presence as key structural units in many natural products and important pharmaceuticals, but their great potential in liquid crystals, and non-linear optical materials<sup>2</sup>.



Pd-catalyzed C-H bond activation is a very powerful tool for C(sp<sup>2</sup>)-C(sp<sup>2</sup>) bond formation, however, direct coupling of olefins is not a general reaction and only a few examples have been reported so far, mostly under no mild conditions.

In this contribution, I will present the preliminary collected results for the oxidative dimerization of styrenes and acrylates to obtain diene, promoted by palladium acetate in ionic liquids. Despite these neoteric media being more and more suggested as ideal substitutes for traditional solvents in catalysis, especially in the field of C-C couplings<sup>3</sup>,

the use of ionic liquids (ILs) in this process has been totally neglected.

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#### BIOGRAPHY

The research carried out by Dr. Monopoli can be traced back to four main themes: a) use of ionic liquids as alternative solvents in organic synthesis and study of their effect on the catalytic activity of metal nanoparticles (palladium, copper, gold, etc ...); b) applications of ionic liquids as solvents for non-catalytic reactions; c) use of catalysts in organic synthesis and green chemistry d) new synthetic approaches for the valorisation of CO<sub>2</sub> and biodiesel production; d) development of innovative analytical protocols (including synthesis of new matrices) for applications in MALDI mass spectrometry.

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4<sup>th</sup> Global Summit on

# CATALYSIS & CHEMICAL ENGINEERING

April 13-14, 2023 | Rome, Italy



## Antonia Iazzetti

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Sacred Heart, L.go F. Vito 1, Rome, Italy

### Advances in transition metal-assisted synthesis and functionalization of heterocycles

**H**eterocycles are motifs of great interest in organic synthesis since they are widespread in a wide range of natural substances, biologically active compounds, and commodity chemicals. For this reason, a great deal of attention is continuously devoted to the development of new protocols to access them.

Transition metal catalysis has been widely employed in the synthesis of heterocyclic rings providing increased functional group tolerance, simplified procedures, and improved yields.

Recently, the construction of heterocyclic systems from benzenoid precursors through cyclization reactions and the functionalization of preformed rings have been studied. Taking advantage of palladium catalysis various class of heterocycles has been obtained and the mechanistic feature of each protocol has been investigated.

This presentation will report on our recent results in this area with the main regard to those protocols based on the use of 2- and 3-acetoxymethylindoles and "soft" nucleophiles.

#### BIOGRAPHY

Antonia Iazzetti is a professor assistant at the Catholic University of the Sacred Heart of Rome, working in the field of organometallic chemistry. Since her Ph.D. in Pharmaceutical Science at the Sapienza University of Rome in 2013, Antonia Iazzetti focused her research activities on the development of new synthetic methods for the construction of polyfunctionalized molecules of biological interest taking advantage of palladium, copper, and gold catalysis. Recently she has aimed at the valorization of industrial by-products by developing innovative and highly sustainable extraction/purification/concentration technology to be applied to the recovery of valuable compounds from production side streams. She is involved in international (Horizon 2020) and national (PRIN 2017) relevant research projects that encouraged her scientific collaborations with various groups.

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## Lucia Steenkamp

CSIR, Chemicals Cluster, South Africa<sup>1</sup>

### Industrial Biocatalysis in South Africa

In South Africa, Bio-economy refers to any biotechnological activities and processes that can result in industrial application and is based on “technological and non-technological exploitation of natural resources”. The natural resources include animals, plant biodiversity, micro-organisms, and minerals to improve human health, address food security and subsequently contribute to economic growth and improved quality of life”. Biocatalysis has been identified as one of the areas in South Africa which will contribute to the Bio-economy.

The vision of the government is for South Africa’s bio-economy to be a significant contributor to the country’s economy by 2030 in terms of the gross domestic product (GDP) and this will involve growing novel industries that generate and develop bio-based services, products and innovations. With the world moving towards a low-carbon economy and decreased pollution, biocatalysis offers the potential to create new green technologies contribute to this vision.

In 2020, the Department of Science and Innovation and the Technology Innovation Agency (TIA) in South Africa identified biocatalysis as an important area to grow the Bio-economy. Following an open selection process to host an Industrial Biocatalysis Hub of

South Africa, the Council for Scientific and Industrial Research (CSIR) was awarded hosting of the Hub. As part of the activities of the Hub, research has to be established in collaboration with large companies and SMME industry partners to develop technologies for commercialization. The model of the Hub is that of a wheel and spoke, and Nodes have been established at several Universities to train researchers that can be employed by the industry partners.

The use of biocatalysis in commercial processes is gaining momentum as the processes can be carried out in organic solvents as well as aqueous environments, with enzymes and biocatalytically active cells. Some of the technologies developed by the CSIR for industry include (S)-naproxen, an anti-inflammatory drug, (-) Ambrafuran and irones for the fragrance industry, L-menthol for the flavours industry, natural extraction of ferulic acid for the food and cosmetics industry and aloesin for the cosmetics industry. A platform technology has also been created for bioconversion of nitro containing substrates to amine products, which with normal chemical synthesis results in explosive reactions. Using biocatalysis, reactions are done near ambient temperatures with no hazardous conditions or outcomes. These examples will be covered in detail.

#### BIOGRAPHY

Dr Lucia Steenkamp is a Principal Researcher at CSIR and Director of the Industrial Biocatalysis Hub in South Africa, specialising in Biocatalysis and has been an author and co-author of numerous peer-reviewed papers and two book chapters. She has developed technologies for industry clients in the pharmaceutical, veterinary, biocides, food, flavours and fragrance industries, leading to five granted patents, nine technology demonstrators and five technology packages licensed to external clients. She has won the South African Women in Science Award (SAWISA) for Research and Innovation in 2018 for her work leading to technologies for commercialisation. She has been a finalist in the NSTF rewards in 2012, 2019 and 2020 for the development of new Green technologies.

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## Laura Scrano

University of Basilicata, Potenza, Italy

### Innovative methods for the recycling and reuse of contaminated water: The Nanowat project

Proposals for the reuse of alternative waters are of growing interest for regions stressed by scarce water availability. Collection, treatment and redistribution are some of the phases that require different purification actions, actions related to the water origin (e.g., grey, rain, and industrial waters).

It is known that wastewater contains both chemical and microbiological contaminants. For this reason, it is essential to have reliable control tools for assessing both risks (chemical and microbiological), for which, often, there is a lack of clear and comprehensive reference standards.

NANOWAT project (Diffusion of nanotechnology-based devices for water treatment and recycling) has focused on developing and diffusion in the Mediterranean area of new technologies for efficient water treatment based on natural and modified nano-

materials, using either filtration and sedimentation, photo-degradation, photocatalysis and their combination.

Pilot-scale mobile equipment for treating different types of wastewater like pesticides, pharmaceuticals, and organic contaminants from industrial enterprises was developed and realized. In detail was carried out the filtration using both nano-structured clay-micelles and clay-vesicles to facilitate the immobilization of organic pollutants, microfibers and micro-plastics and successively on the recalcitrant compounds, still contained in the liquid phase after filtration treatment, were performed new photo-catalytic processes based on TiO<sub>2</sub> in suspension and on immobilized on glass. The results were exciting and compelling, confirming the need to customize the wastewater purification procedure concerning the type of contamination present.

#### BIOGRAPHY

Associate Professor SSD AGR/13. Visiting professor IUT, University Claude Bernard, Lyon 1, France ANVUR disciplinary expert. Qualified as Full Professor SSD AGR/13. Prof. Scrano has been a co-proposer in four national and international research projects, and she coordinated one of them. She is the author/co-author of many scientific articles published in international referenced journals (indexed Scopus) and of several scientific papers published in national journals and national and international conference proceedings, in two of which she has obtained a prize for the scientific activity developed.

Prof. Scrano studies the properties that allow some clay minerals to retain organic molecules present in the soil, including some herbicides of the latest generation, and how the constituents of the soil (organic matter and clay minerals) influence the degradation process..

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## Yongdan Li

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### Challenges and progresses of large-scale electric energy storage with flow electrochemical reactors

The development of renewable and distributed energy systems calls for large scale energy storage technologies. In recent years, a blooming of the energy storage technologies, e.g., various configurations of flow and hybrid batteries, different concepts of electrolysis cells, as well as diverse designs of fuel cells, is experienced. This presentation will give an overview of the dynamic and prosperous energy storage technologies based on flow reactors, which promise an as large as the grid scale energy storage. After proposing a perspective of the field, the presentation will focus on the recent progresses on the following two topics:

Redox flow battery (RFB) is one of such promising energy storage technologies owing to its independent power and energy features, long cycle life, and rapid response. The aqueous RFBs

have been already demonstrated, while the non-aqueous RFBs (NARFBs) have received increasing attention because of their wide electrochemical window and thus high energy density. This presentation will disclose the research on the highly selective and conductive membranes and the design of the active molecules both for anolyte and catholyte.

Lithium oxygen battery with Li<sub>2</sub>O as the discharge product has a theoretical specific energy density as high as 5200 Wh kg<sup>-1</sup>, which is superior to the state-of-the-art lithium ion batteries. Our recent work on the design of cathode catalyst allows to achieve this discharge state with extremely high reaction rate. A stable low charge-discharge overpotential 50 mV with a high energy efficiency (EE) 98.2% at 0.1 mA cm<sup>-2</sup> for over 100 cycles was enabled with this device.

#### BIOGRAPHY

Yongdan Li, Chair Professor of Industrial Chemistry of Aalto university, Finland. He received his Ph.D. degree in Chemical Engineering from Tianjin University, China in 1989. In 1993, he became a full Professor of Industrial Catalysis in Tianjin University. In 2017, he joined Aalto university as a tenured full professor. His research interests include photocatalytic hydrogen production, devices for large scale energy storage and conversion, biomass conversion to fuels and chemicals and NO<sub>x</sub> abatement in flue gas. He was the Changjiang Chair Professor of Industrial Catalysis in Tianjin, China. He is now the coordinator of the EU Horizon 2020 EHL CATHOL project and a partner of the Horizon EU EPOCH project. He is also the PI of an Academy of Finland project, the MEMBAT.

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4<sup>th</sup> Global Summit on  
**CATALYSIS &  
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April 13-14, 2023 | Rome, Italy

**Scientific Sessions**

**Day 2**

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**CHEMICAL CATALYST 2023**



## Fast oxygen reduction and evolution kinetics enabled by $\text{LaNi}_{0.5}\text{Co}_{0.5}\text{O}_3$ perovskite cathode for a molten salt $\text{Li-O}_2$ battery

**Qianyuan Qiu and Yongdan Li**

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Rechargeable lithium-oxygen ( $\text{Li-O}_2$ ) batteries have been regarded as a promising energy storage device, but its practical use is impeded by its low energy efficiency. The underneath reason is the sluggish reaction kinetics at the cathode side, where oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) take place during the discharge and charge step, respectively. The lack of efficient catalysts hinders the cathode reaction and thus leads to undesired electrochemical performance. Perovskite oxide have been widely investigated as bi-functional catalysts for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) in other energy devices, e.g. solid oxide fuel cell. It usually exhibits high electronic conductivity, oxygen affinity and catalytic activity

towards oxygen species. Herein, a bi-functional catalytic perovskite  $\text{LaNi}_{0.5}\text{Co}_{0.5}\text{O}_3$  (LNCO) is employed as the cathode of an efficient  $\text{Li-O}_2$  battery with a molten nitrate salt electrolyte at 160 oC. It displays a stable low charge-discharge overpotential 50 mV with a high energy efficiency (EE) 98.2% at 0.1  $\text{mA cm}^{-2}$  for over 100 cycles. The excellent performance is attributed to the extremely fast oxygen reduction and evolution kinetics on the surface of LNCO. The discharge product is  $\text{Li}_2\text{O}$  with a porous and fluffy morphology which facilitates the transfer of oxygen and other intermediate species. It is noted that  $\text{Li}_2\text{O}$  as a discharge product enables a theoretical specific energy density of 5200  $\text{Wh kg}^{-1}$ , which is superior to the  $\text{Li}_2\text{O}_2$  as product giving 3500  $\text{Wh kg}^{-1}$  for those ambient temperature  $\text{Li-O}_2$  batteries.

### Biography

Qianyuan Qiu, a PhD student from Aalto university, Finland. She received her M.S. in green energy chemistry and technology from South China University of Technology in 2016. Her research interests include energy storage and conversion devices, such as lithium batteries and solid oxide fuel cells.

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## Rational design of catalysts for efficient CO<sub>2</sub> activation

**Patricia Concepción<sup>1</sup>, Jaime Mazarío<sup>1</sup>, Pablo G. Lustemberg<sup>2,3</sup>, M. Verónica Ganduglia-Pirovano<sup>2</sup>, Marcelo E. Domine<sup>1</sup>, Carmen Tébar-Soler<sup>1</sup>, Vlad Martin Diaconescu<sup>4</sup>, Laura Simonelli<sup>4</sup>, Alexander Missyul<sup>4</sup>, Jose Juan Calvino<sup>4</sup> and Avelino Corma<sup>1</sup>**

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**D**ecarbonisation of the energy sector to reach net zero greenhouse gas emission requires multiple actions, including electrification of the power sector, increasing energy efficiency, promoting a circular economy, and developing carbon capture, utilization and storage technologies. This talk is focused on improve energy efficiency in the frame of carbon utilization technologies, in particular

in the synthesis of methanol and methane. Overcoming the complexity of catalysts by a rational synthesis of new catalysts and decreasing reaction temperature while keeping high catalyst efficiency request a fundamental knowledge of active sites. In this talk, we will report a rational design of catalysts where operando spectroscopic tools play a key role in the identification of active species and reaction mechanism.

### Biography

Dr. Patricia Concepcion belongs to the Higher Council for Scientific Research of Spain (CSIC), where since 2002 she works as researcher at the Institute of Chemical Technology in Valencia (Spain). Her research cover heterogeneous catalysis, sustainable processes, CO<sub>2</sub> valorization, and operando spectroscopy. The goal of her work is to determine structural- activity correlations of solid catalysts with applications in industrial relevant reactions. She is author or co-author of over 200 publications, has 7 patents and two book chapters.

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## Carbon spheres modified with APTES (aminosilane) for CO<sub>2</sub> capture

**Ewelina Kusiak-Nejman<sup>1\*</sup>, Marta Prochowska<sup>1</sup>, Filip Latzke<sup>3</sup>,  
Joanna Kapica-Kozar<sup>1</sup>, Ewa Ekiert<sup>1</sup>, Iwona Pelech<sup>1</sup>,  
Antoni W. Morawski<sup>1</sup>, and Urszula Narkiewicz<sup>1</sup>**

*West Pomeranian University of Technology in Szczecin, Faculty of Chemical Technology and Engineering,  
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Carbon capture and storage (CCS) processes are classified as the key technologies to effectively reduce carbon dioxide mainly from industrial sectors. Budinis et al. [Energy Strategy Reviews 22 (2018) 61-81] deduced that in the medium (up to 2050) and long (up to 2100) terms predictions including CCS result in 37% and 65% of fossil fuel reserves being consumed, respectively.

This work aimed a one-step method of carbon spheres preparation and modification utilizing (3-aminopropyl)triethoxysilane as a catalyst and modifying agent at the same time. Carbon dioxide adsorption was measured at 0 and 25°C involving a QUADRASORB evoTM gas sorption automatic system (Quantachrome Instruments, USA) and at 30-60 °C using STA 449 F3 Jupiter thermobalance (Enrich NETZSCH GmbH & co. Holding KG, Germany). The presentation will

discuss the adsorption properties of the materials obtained in relation to their structural and morphological properties (e.g. the presence of APTES functional groups on the carbon spheres surface or the carbon sphere size before and after modification). The proposed mechanism of carbon spheres formation using aminosilane instead of ammonia water solution will be discussed as well. Both the method of obtaining carbon spheres and the type of modifying agent used, represent a scientific novelty in terms of investigating the sorption capacity of these materials towards CO<sub>2</sub>.

**Acknowledgements:** The research leading to these results has received funding from the Norway Grants 2014-2021 via the National Centre for Research and Development under the grant number NOR/POLNORCCS/PhotoRed/0007/2019-00.

### Biography

Dr. Ewelina Kusiak-Nejman is an Associate Professor at West Pomeranian University of Technology in Szczecin, Poland. She has been working in the field of photocatalytic water treatment and air purification utilizing modified TiO<sub>2</sub> and other semiconductors deposited on various carbon structures, e.g. activated carbon fiber and carbon spheres. Her publication output includes over 80 JCR-listed publications. Currently, Dr. Kusiak-Nejman is co-implementing the research project "Photocatalytic and photoelectrochemical reduction of carbon dioxide" in cooperation with Norwegian partners: University of South-Eastern Norway, SINTEF AS Industry and SINTEF AS Ocean.

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## Performance improvement of electrospun membranes for water treatment by coupling AOPs with composite catalytic systems

**Carlo Boaretti, Martina Roso, Alessandra Lorenzetti  
and Michele Modesti**

*University of Padova, Italy*

The use of advanced oxidation processes (AOPs) for the removal of organic contaminants in wastewater has drawn great attention as a promising solution to limit environmental pollution but still suffers from limitation towards widespread employment. This work presents an effort towards the enhancement of the performance of such processes, combining their use with electrospun composite membranes to develop highly efficient mixed catalytic heterogeneous medium for water treatment. To such end the photo-activity of TiO<sub>2</sub> towards the decolorization of methyl orange (MO) was improved by the combination with Fe<sub>3</sub>O<sub>4</sub> particles synthesized by co-precipitation and employed as heterogeneous Fenton catalyst. A third system was realized by the combination of such catalysts with graphene oxide (GO) to promote surface absorption and mediate

electron-transfer reaction. All the catalytic systems were deposited on PVDF nanofibers used as support to provide mechanical and UV resistance. Along with such membranes different AOPs strategies were investigated either alone or in combination using UV radiation, ultrasounds and H<sub>2</sub>O<sub>2</sub>, evaluating the relative performances using a batch configuration mode. The results revealed that while photocatalysis, sonophotocatalysis and Fenton reaction alone have a limited efficiency towards MO decolorization their proper combination dramatically increased the kinetic of the process with a better performance in presence of GO. Such combined effect allowed to obtain a complete decolorization of 10 ppm of MO in less than 20 mins with the employment of only 1 ppm of H<sub>2</sub>O<sub>2</sub> and good membrane activity over several degradation cycles.

### Biography

Carlo Boaretti is currently researcher at the Department of Industrial Engineering of the University of Padova. He graduated in Chemical and Industrial Process Engineering in 2012. He defended his PhD in Industrial Engineering in 2016 with a thesis related to the applications of electrospun nanofibers for energy and environmental applications with specific focus on the application of different approaches to improve the photocatalytic performance of nanostructured membranes. During his post-doc he joined the Polymer Engineering Group of Padova University in several national and international projects on the development of polymer functional materials. His actual research interests are related on the application of alternative energy sources (ultrasound, UV and microwaves) to chemical processes and on the recycling of polymeric materials.

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## Designing Purpose-Built Ligands for Catalysts: "Say Live and Let Die...."

**Michael G. Organ**

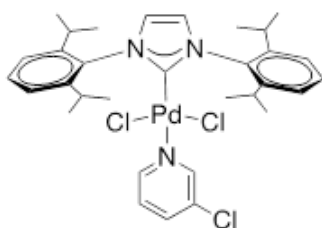
*Director of the Centre for Catalysis Research and Innovation, uOttawa*

This seminar will address the invention and evolution of the Pd-PEPPSI catalyst platform (PEPPSI = pyridine enhanced pre-catalyst preparation stabilization and initiation).

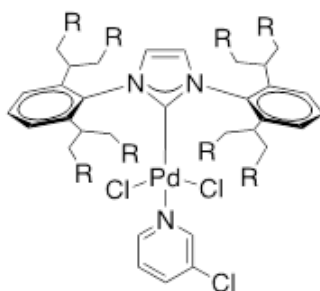
Considerable effort for almost half a century has been devoted to understanding how ligand steric and electronic properties modulate the reactivity of a metal centre in a large number of catalytic processes. This is confounded by the fact that many of these transformations have two or more steps in their catalytic cycles, which may mean that a favourable attribute in one step may act to disfavour another step. Many groups have worked diligently to develop methods to probe, and scales to grade ligand properties such that they can be used in, ideally, a predictive fashion

to guide the development of new catalysts.

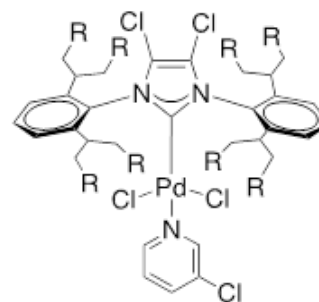
In this presentation our approach to rational ligand design in cross-coupling applications will be discussed and how this approach has been used to improve catalyst performance in terms of both general reactivity and selectivity. In particular, time will be dedicated to the discussion of 1) avoiding beta hydride elimination in the coupling of alkyl nucleophiles and electrophiles leading to metal hydride formation and olefin byproducts, 2) the incorporation of secondary alkyl centres onto aromatic and heteroaromatic cores without isomerization to create more architecturally complex molecular targets, and 3) the impact of these innovations in drug discovery and materials science.



**Pd-PEPPSI-IPr**  
(First Generation)



**Pd-PEPPSI-IPent (R = Me)**  
**Pd-PEPPSI-IHept (R = Et)**  
(Second Generation)



**Pd-PEPPSI-IPent<sup>Cl</sup> (R = Me)**  
**Pd-PEPPSI-IHept<sup>Cl</sup> (R = Et)**  
(Third Generation)

## Biography

Dr. Organ received his PhD in 1992 at the University of Guelph under the tutelage of Professor Gordon L. Lange. He then was an NSERC Postdoctoral Scholar in the laboratory of Professor Barry M. Trost at Stanford (1994). His independent career started at Indiana University-Purdue University at Indianapolis in 1994 after which he moved in 1997 to York University in Toronto where he rose through the ranks to full professor. Effective January 2016, he is the Director of the Centre for Catalysis Research and Innovation (CCRI) at the University of Ottawa.

His group pioneered the concept of microwave-assisted, continuous flow organic synthesis as well as several unique technologies that underpin these efforts. These include new microwave applicator design, metal-film coated flow reactors to promote organic transformations, extreme temperature and pressure reactor and process design, continuous in-line analysis, and hands-free, intelligent process optimization and monitoring using in-house created software. In 2020, these efforts led to flow technology used directly for the commercial manufacture of a key organic molecule used to prepare billions of COVID-19 test kits (<https://www2.uottawa.ca/about-us/media/news/little-goes-long-way-uottawa-research-team-plays-key-role-global-detection-covid-19>).

His group's effort in catalysis has led to the creation of a broadening series of N-heterocyclic carbene (NHC)-based organometallic complexes that have shown unsurpassed reactivity and selectivity in a wide number of cross-coupling applications. This family of catalysts (coined PEPPSI for pyridine-enhanced precatalyst preparation, stabilization, and initiation) has been commercialized and is used widely including at scale in the commercial manufacturing of active pharmaceutical ingredients (API).

Dr. Organ is an SFI Walton Fellow (2002), a Xerox Foundation Fellow (2007), a Merck-Frosst Canadian Academic Development Program Fellow (2007), the Naeja Pharmaceuticals Lecturer at University of Alberta (2008), a JSPS Fellow (Japan, 2010), an Agilent Laboratories Fellow (2011), and was awarded an NSERC Accelerator Supplement (2013). In 2016 he was awarded the Raymond U. Lemieux Award for Organic Chemistry by the Canadian Society for Chemistry. In 2017 he was awarded the Encyclopedia of Reagents for Organic Synthesis (EROS) 2017 "Best Reagent Award". Dr. Organ received the NSERC John C. Polanyi Award in 2018, given to an individual or team whose research has led to a recent outstanding advance in any field of the natural sciences or engineering. In 2021, he was awarded "The Catalysis Award" by the The Chemical Institute of Canada.

Professor Organ's research on the structure of alkyl- and aryl organozincs as it relates to the mechanism of Negishi Reaction was called "one of the most Notable Discoveries in Synthetic Chemistry in 2014" by Chemical and Engineering News. Dr. Organ and his research career were profiled in *Angewandte Chemie* (2013).

He started and has run two spin-out companies successfully since 1998.

Dr. Organ was appointed to the international advisory boards of ACS Combinatorial Science (2002), *The Journal of Flow Chemistry* (2011), *Chemistry, A European Journal* (2013) and *ChemCatChem* (2016).

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## The use of CO<sub>2</sub> as a building block

**Timo Repo, Jere Mannisto, Aleksi Sahari, Jukka Puumi and Teemu Niemi**

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Efficient methods to activate C-O bonds and use of CO<sub>2</sub> as a C1-building block are attractive and sustainable pathways for synthesis of highly valuable pharmaceuticals, chemicals and materials from which our modern society is depending on. Herein heterocycles were selected as target compounds. For example, whereas cyclic carbonates are widely used as aprotic polar solvents and synthetic intermediates, while 5-membered carbamates (2-oxazolidinones) find their importance in antibiotics.

In general, possibility to generate a carbamate anion and use its ability to undergo nucleophilic attack opens a generic approach to synthesis of broad range of cyclic carbamates, including highly important 2-oxazolidinones.[3-4] Recently, we

have focused on the synthesis of  $\gamma$ -butyrolactones using Grignard reagents, CO<sub>2</sub> and aldehydes as building blocks[5], and for synthesis of O-aryl carbamates from aryl iodides or bromides, amines and carbon dioxide [6].

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3. For a review, see: Niemi, T. et al, Eur. J. Org. Chem. 2019, 1180.
4. Sahari, A. et al, Chem Commun. 2022, 58, 3027-3030.
5. Sahari et al., Submitted.

### Biography

Timo Repo received his PhD in 1997 from University of Helsinki (Finland), where he was nominated as a full professor of inorganic chemistry in 2007. His research is focused on green chemistry and homogeneous catalysis, including catalyst development for activation of small molecules (e.g. O<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub>), oxidation, reduction, C-H activation, and biomass valorization. He has published around 190 scientific publications.

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## Direct biogas methanation on Ni/CeO<sub>2</sub> catalysts obtained from soft-templated mixed oxides

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<sup>2</sup>*Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM), Italy*

**B**iogas, mainly composed of methane and carbon dioxide (together with nitrogen, oxygen, hydrogen sulfide and other contaminants), is one of the most promising sources of renewable energy. It can be upgraded to high-quality “renewable natural gas”, with a high content (> 90%) of biomethane, by removing CO<sub>2</sub>, even without its reuse. However, converting the large amount of CO<sub>2</sub> into CH<sub>4</sub> – using renewable hydrogen – would make biogas valorization more attractive. Even better, performing CO<sub>2</sub> methanation directly in the biogas stream would simplify the process, avoiding the use of expensive separation technologies.

The direct methanation of CO<sub>2</sub> contained in a model biogas was investigated on a series of Ni/CeO<sub>2</sub> catalysts. NiO/CeO<sub>2</sub> nanostructured mixed oxides were synthesized by the soft-template

procedure with different Ni/Ce molar ratios. The samples were thoroughly characterized (by ICP OES, XRD, (HR-)TEM, N<sub>2</sub> physisorption, and H<sub>2</sub>-TPR) and then reduced in H<sub>2</sub> prior to catalytic testing. The ability of the H<sub>2</sub> treated samples to adsorb the reactants was also investigated, by means of CO<sub>2</sub> adsorption microcalorimetry and H<sub>2</sub>-pulse chemisorption measurements. Methanation tests were carried out in a tubular fixed bed microreactor, at atmospheric pressure, with a CO<sub>2</sub>/CH<sub>4</sub>/H<sub>2</sub> (molar ratios 1/2/4) feed. Besides the effect of catalyst composition and properties, that of temperature and space velocity was also investigated. Since high methanation activity was obtained even at mild reaction conditions, a remarkable enhancement is expected by a further optimization of the operating parameters, especially in terms of pressure.

### Biography

Graduated in Chemistry in 1996 at the University of Cagliari, she soon joined the research group in Industrial Chemistry with a research contract. In 2003 she got her PhD in Chemistry. After a one-year post-doc fellowship at Tulane University (New Orleans, USA), she went back to Cagliari with a research contract. In 2006 she became an Assistant Professor and she is now an Associate Professor of Industrial Chemistry. She teaches Industrial Chemistry (Degree in Biotechnologies) and Ecosustainable Industrial Processes (Master Degree in Chemical Sciences). Her research activity has been mainly developed in the field of heterogeneous catalysis. Recent interests include purification of hydrogen, production of fuels and fine chemicals from renewable materials, and chemical recycling of CO<sub>2</sub>.

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## Platinum Catalysts for the Lignin Conversion into Phenolics as Bio- based Resource for Phenolic Resins

**Ilaria Longobardo<sup>1</sup>, Gisa Meissner<sup>1</sup>, Hendrik Spod<sup>1</sup>,  
Raphaela Suess<sup>2</sup> and Birgit Kamm<sup>2</sup>**

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With our presentation we would like to highlight strategies to obtain organic phenolic building blocks to produce biobased phenolic resins from biomass using precious metal-based catalysts. For the investigations, various platinum-based catalysts were synthesized using different impregnation methods. Here, we studied platinum-based catalysts for the efficient formation of phenolics from lignin as bio-based building blocks with end use as phenolic resin. The catalyst performance depends on the used precious metal (PM) precursor solutions, e.g., platinum nitrate, hexachloroplatinic acid or platinum oxalate and on intrinsic characteristics of the support. Especially, the special nature of a hydrotalcite (HTC) as support material shows positive effects the catalyst performance. A higher platinum loading leads to a full lignin conversion, which

can be explained by an increased PM surface area, resulting in a higher catalyst activity. Also, the higher the platinum-loading of the catalyst, the higher the preference towards the formation of monomeric and oligomeric structures. The addition of 1% Nickel even strengthens this effect with a decreased coke formation. Afterwards, the reactions conditions were optimized based on a design of experiment (DoE) with the successful avoidance of any coke formation.

The PM recovery plays a key role from both an ecological and economical point of view. The full "PM loop" consists of the PM winning and PM solution production as well as the catalyst synthesis, followed by the performance as active catalyst. Finally, the deactivated catalyst is separated from the reaction mixture to close the loop with the PM recycling, which serves again as PM source.

### Biography

Ilaria Longobardo is a sales manager at Heraeus Precious Metals. She has been working for Heraeus since 2017 where she started the dual studies programs with the aim of achieving the degree of Master of Science in Business administration. In these five years she was able to deepen her knowhow regarding precious metals catalysis and recycling. In 2020 Ms. Longobardo started working in the field of heterogeneous catalysis by joining an Heraeus internal startup which focuses on delivering core materials for the hydrogen economy. Afterwards she further focused on catalysis by joining the Heraeus emission and chemical catalysts team where she drives the expansion of the heterogeneous precious metal catalyst product portfolio by building strong technical relationships with key customers.

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## Re-treated zeolites for the HOCK rearrangement in the cumene process

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<sup>2</sup>*Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Aachen, Germany*

With  $12.7 \times 10^6$  t worldwide produced annually, phenol is one of the most important organic commodity chemicals. [1] To produce phenol, the Hock process is still the by far most used process today [2]. One crucial step of this process is the cleavage of cumene hydroperoxide (CHP), known as Hock rearrangement, which has a major impact on the overall cumene consumption rate of the entire phenol process. The most commonly used catalyst for the cleavage of CHP is sulfuric acid [3], which unfortunately has intrinsic disadvantages: in addition to corrosion issues, it is necessary to add a neutralizing agent to the reaction mixture after the decomposition of CHP has taken place to prevent side reactions. Furthermore, removing the aggressive acid before rectification is required. A way to reduce energy consumption and waste production of the process is to substitute sulfuric acid with heterogeneous catalysts.

In our study, we investigated LTX zeolites as catalysts for the Hock-cleavage. A high catalytic activity was achieved with LTX zeolites calcinated at high temperatures. XRPD analyses indicate major changes in the crystal structure after temperature treatment at 900 °C or higher. XRF analysis concerning the surface Si/Al-ratio of these materials lead the assumption of the formation of extra framework aluminum, which could be responsible for the high catalytic activity. The newfound material shows potential to be an alternative to sulfuric acid for the HOCK rearrangement.

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### Biography

2007 – 2009 PhD thesis in Technical Chemistry at RWTH Aachen with Prof. Dr. W.F. Hölderich

2010 – 2014 Laboratory head with Oxea Chemicals, chemical park Ruhrchemie, Oberhausen

Since 11/2014 Professor for Chemical Technology at TH Köln University of Applied Sciences.

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# About Rome

Rome, Italian Rome, historic city and capital of the province of Rome, the region of Lazio and the country of Italy. Rome is located in the central part of the Italian peninsula, on the Tiber, about 15 miles inland from the Tyrrhenian Sea. The province of Rome serves as a setting for the many treasures of the capital, and the surroundings have, more or less directly, been influenced by the history of the Eternal City. A region that has a lot to offer: sea, nature, gastronomy and villages rich in history and art. Sea, hills, lakes, rivers and vineyards: the surroundings of Rome offer a kaleidoscope of diversity and attractions for nature lovers.

## **Are you coming to Rome in April?**

You will enjoy mild weather, lots of flowers and a bustling city full of life with lots of activities, both indoors and outdoors.

## **Interesting Facts about Rome:**

Modern Rome has 280 fountains and over 900 churches. Nearly 700,000 euros worth of coins are thrown into the Trevi Fountain in Rome every year. Profits are donated to Caritas to help people in need. The Romans had built a road network of 53,000 miles by the start of the 4th century. Each Roman mile was approximately 4,800 feet and marked with a milestone, giving rise to the saying "All roads lead to Rome".

Rome's mascot is a she-wolf who cared for the brothers Romulus and Remus, the mythological founders of Rome. Rome became the capital of unified Italy in 1870, taking the title from Florence. Emperor Trajan built the very first trading center in Rome between 107 and 110 AD. He sold a wide variety of merchandise and groceries. Rome's first university, La Sapienza, founded in 1303 AD, is the largest in Europe and the second largest in the world.

Rome has a museum entirely dedicated to pasta. St. Peter's Basilica inside Vatican City is the largest church ever built.





4<sup>th</sup> Global Summit on  
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**Day 2**

(Room-2)

**CHEMICAL CATALYST 2023**



## Chantal Guillard

Université de Lyon, Institut de Recherches sur la Catalyse et l'Environnement de Lyon, UMR 5256, CNRS, Université Claude Bernard Lyon 1, 2 avenue A. Einstein, 69626 Villeurbanne, France

### Can the photocatalytic process contribute to our energy and environmental concerns?

**E**nergy crisis, global warming, lack of water, three scourges of our modern society that it is important to quickly consider. A large number of publications deal with the photocatalytic process as an effective, inexpensive process for simultaneously eliminating pollution from aqueous and gaseous effluents, generating hydrogen and upgrading biomass. What is it really?

The first part of our presentation will deal with environmental applications. Are bacteria, viruses and other microorganisms effectively inactivated by photocatalysis? In particular, we will present results obtained using luminous textiles as a

support. How to solve the problem of generated by-products, harmful for the environment? The coupling of photocatalysis with other processes will then be discussed, such as adsorption, oxidants (ozone, H<sub>2</sub>O<sub>2</sub>), catalysis, plasma. In this part will also be considered the efficiency of the photocatalytic process under visible light.

The second part of our presentation will concern the recovery of aqueous effluent and in particular biomass. Production of H<sub>2</sub>, generation of high value-added products, how effective? impact of the coupling of photocatalysis with catalysis, electrocatalysis, what perspectives?

#### BIOGRAPHY

Chantal Guillard, is chemical engineer. In 1989, She became Doctoc-ès-Sciences in Catalysis of University of Lyon, France. She enters to CNRS the same year to work in Photocatalysis.

Now she is CNRS Director at Institut of Researches on Catalysis and Environment.

She is the authors of 203 papers, 281 communications and 8 patents center on Photocatalysis. Her H-factor is 56. Her studies on photocatalysis field are devoted to fundamental researches to better understand the efficiency and mechanisms of photocatalytic reaction in water and air treatment and on energy and valorization of biomass. She coupled photocatalysis with other process, developed new photocatalytic materials in particular photocatalytic optical fiber fabrics, worked with microbiologists to improve the knowledge on the inactivation of microorganisms.

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## Giuseppe Bonura

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### Direct hydrogenation of CO<sub>2</sub> into DME: catalytic and technological aspects

CCU-related technologies can represent challenging strategies suitable to explore new concepts and opportunities for catalytic and industrial development. In this view, the production of dimethyl ether (DME) from the direct catalytic hydrogenation of CO<sub>2</sub> appears as a viable approach, able to meet also the ever-increasing need for alternative environmentally-friendly fuels and energy carriers. Although several papers document a relatively high productivity on catalytic systems prepared by simple mixing between a methanol catalyst and an acidic matrix, the need for a relatively higher degree of interdispersion among the components is boosting the scientific interest towards the integration of a multi-functionality necessary for reaction within a single catalyst, so to realize a more efficient mass transfer of methanol formed on metal-oxide sites

to the acid sites. This lecture will be focused on the performance of hybrid CuZnZr-zeolite catalysts, tested in a fixed bed reactor under direct CO<sub>2</sub>-to-DME hydrogenation conditions (i.e., TR, 200-260 °C; PR, 3.0 MPa; CO<sub>2</sub>/H<sub>2</sub>, 1/3 v/v). Particular attention will be addressed on the clues related to the reaction mechanism with the aim to ascertain the controlling step preventing the achievement of high CO<sub>2</sub> conversion per pass below 220 °C. The audience will have also the opportunity to learn more about the technological aspects associated to the direct production of DME, suggesting possible solutions for a sustainable process chain. On the whole, people working in this field will acquire new information addressing a practical solution to a serious environmental and economical problem linked to the management of CO<sub>2</sub> emissions in atmosphere.

#### BIOGRAPHY

Giuseppe BONURA is currently a Senior Researcher of the National Research Council (CNR) at the Institute for Advanced Energy Technologies "Nicola Giordano" (ITAE), in Messina, Italy. His scientific interests are in the field of industrial chemistry, with a main focus on the design and development of multi-functional catalytic systems for the production of clean alternative fuels. He is currently involved in various EU and national research projects dealing with CCUS and Power-to-Gas technologies. In addition to numerous national and international conferences and seminars, he has already contributed to the production of over 300 scientific works, including publications in International papers, communications at conferences and technical-scientific reports related to contractual activities with small, medium and large enterprises.

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## Julien Vieillard

Normandie Univ, CNRS, INSA Rouen, UNIROUEN, COBRA  
(UMR 6014 and FR 3038), 55 rue saint Germain, 27000 Evreux

### Surface modification of lignocellulosic material for adsorption and photocatalysis

Organic and inorganic pollutants coming from anthropogenic activity may accumulate in the environment due to water contamination. Adsorption on solid surface and heterogenous photocatalysis have been described as a promising alternative to conventional water treatment. In this communication, we will present how some lignocellulosic agrowastes could be modified and then applied as an adsorbent or a photocatalyst to remove or eliminate respectively different pollutants in water. Different processes of surface modification based on carbonization, hydrothermal treatment but also impregnation

and covalent grafting will be discussed and their performances in adsorption and photocatalysis will be demonstrated.

In addition, this communication also discusses the stabilization of metallic nanoparticles or metallic oxides in lignocellulosic matrices or their derivatives and their ability to degrade the organic pollutants previously adsorbed in the material. We will also discuss the dependence of adsorption and photocatalysis performance mainly on the structure, chemical composition and morphology as well as environmental variables such as temperature, pH and ionic strength.

#### BIOGRAPHY

Dr. Julien Vieillard is a lecturer at Normandy university in France. He worked in COBRA laboratory which is expert in organic and analytical chemistry. Dr Julien Vieillard is an expert in analytical chemistry to develop original biosensors. He also worked on surface modification of polymer and lignocellulosic material. His recent works focused on pollutant removal from water by adsorption and catalysis. Dr. Julien Vieillard participated to 53 articles published in international journal.

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## Piotr Cyganowski



Department of Process Engineering and Technology of Polymer and Carbon Materials, Wrocław University of Science and Technology, Wyb. S. Wyspiańskiego 27, 50-370 Wrocław, Poland

### The powerful response for the major environmental threats. The catalytic hydrogenation of aromatic nitro compounds over rhenium-based nanocatalysts

**E**nvironmental hazards arising from the occurrence of nitroaromatic compounds (NACs) are recognized as one of the major challenges of the modern chemical engineering. NACs, such as unsubstituted nitrobenzenes, nitroanilines, and nitrophenols are toxic, and mutagenic, and still, they belong to the largest group of chemicals used on an industrial scale. In this context, there is a pressing need for the development of new and efficient ways enabling overcoming the negative impact that NACs cause. One of them is the process of catalytic hydrogenation over metallic nanoparticles (NPs). This nanotechnology-based approach is particularly important, as it allows, on the one hand, to deactivate NACs under mild conditions, and on the other hand, enables production of aromatic

amines, that are recognized as fine chemical products for the i.a. pharmaceutical industry.

**U**p to date there is a number of nano-catalysts applied for the hydrogenation of NACs. This includes various nanomaterials, however these based on NPs of precious metals (e.g. Au, Pt, Pd) offer extraordinary catalytic activities and high NACs reduction yields (%). In this context, the present studies propose a new and emerging nano-catalysts based on ReNPs. Re offers unique and universal catalytic chemistry, and the wide spectrum of catalytically active Re species, makes the nanomaterials based on thereof, an universal tool for the deactivation of NACs and the production of their amino-analogues. This further led to increasing catalytic activity in the NACs hydrogenation processes.

#### BIOGRAPHY

Prof. Piotr Cyganowski is an Associate Professor at Wrocław University of Science and Technology. He earned his PhD in Physicochemistry of Macromolecular Compounds in 2017, and his DSc degree in Chemical Engineering in 2022. He carries out his activities as a part of research projects financed by the National Science Center (Poland), as well as in the cooperation with industrial units. In his research, he focuses on the development of new separation materials based on anion exchange resins as well as the innovative methods for the synthesis of catalytic materials with transition group metals nanoparticles. Dr Cyganowski is also the laureate of the scholarship program for outstanding young scientists under the auspices of Polish Ministry of Education and Science.

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## B. Frank Gupton, *Ph.D.*

Floyd D. Gottwald Chaired Professor  
Department Chair, Department of Chemical and Life Science  
Engineering under of the Medicines for All Institute

### Novel Carbon Support Systems for Palladium Catalyzed Cross Coupling Reactions

**E**nvironmental hazards arising from the occurrence of nitroaromatic compounds (NACs) are recognized as one of the major challenges of the modern chemical engineering. NACs, such as unsubstituted nitrobenzenes, nitroanilines, and nitrophenols are toxic, and mutagenic, and still, they belong to the largest group of chemicals used on an industrial scale. In this context, there is a pressing need for the development of new and efficient ways enabling overcoming the negative impact that NACs cause. One of them is the process of catalytic hydrogenation over metallic nanoparticles (NPs). This nanotechnology-based approach is particularly important, as it allows, on the one hand, to deactivate NACs under mild conditions, and on the other hand, enables production of aromatic

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#### BIOGRAPHY

Dr. Frank Gupton is a professor at Virginia Commonwealth University and holds joint appointments in the Departments of Chemistry and the Department of Chemical and Life Science Engineering. He is the Floyd D. Gottwald Chair of Pharmaceutical Engineering and also serves as Department Chair of the Chemical and Life Science Engineering Department. His thirty-year industrial career centered on the development and commercialization of chemical processes for pharmaceutical applications. Dr. Gupton's research group is currently focused on the development of continuous processing technology to facilitate the discovery, development and commercialization of drug products.

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## Scientific Sessions

### Day 2

(Room-2)

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## Regeneration of coked catalysts used in plastics pyrolysis: ozonation as an alternative process to oxygen oxidation

**Vivien Daligaux, Romain Richard and Marie-Hélène Manero**

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Industrial regeneration of coked catalysts is mainly conducted by oxidation under air or oxygen at high temperatures (400-600°C). Due to the high oxidative power of ozone, coke removal by ozonation appears as a promising alternative method to achieve catalysts regeneration at lower temperatures (around 100°C). For this study, catalytic pyrolysis of polyethylene is carried out with HZSM-5 zeolites as catalysts, this reaction being identified in the literature as a high-interest reaction for plastic waste revalorization whose industrial application is limited due to an important deactivation via coke formation. Ozonation process for coke removal from obtained deactivated zeolites is processed in a fixed-bed reactor and the influence of different operating parameters is studied (temperature, O<sub>3</sub> concentration, flow-rate and time-on-stream). Coked and partially

regenerated samples are analyzed with various analytical techniques (CHN analysis, N<sub>2</sub> adsorption, <sup>13</sup>C RMN) to determine the evolution of zeolite properties as well as coke amount and nature. Promising results are obtained with a maximum carbon removal of 90% from an initial carbon content of 7.8 wt.%C in the coked sample exposed to a mixed oxygen/ozone gas flow (50 g/Nm<sup>3</sup> of ozone at 50 L/h) during 10h at 100°C. Experimental results show similar behavior to oxygen oxidation as reactivity follows shrinking-core model with a progressive coke removal from pellet outer-shell towards its core. Influence of operating parameters are discussed, allowing a better comprehension of diffusion limitations generated by the competition between ozone reactivity with coke and ozone thermal and catalytic decomposition.

### Biography

After graduating from engineering school (INSA Rouen, France), Vivien Daligaux integrated "Laboratoire de Génie Chimique" (LGC Toulouse, France) as a PhD student in October 2020. His PhD thesis work "Ozonation process for coked catalysts regeneration" is carried out in the current lab under the supervision of Marie-Hélène Manero and Romain Richard. From previous experiences during internships, he had the opportunity to discover both industrial research (Total and Air Liquide, France) and to work in a lab abroad (CSIRO, Clayton, Australia) which led to the wish of pursuing research with a PhD.

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## Catalytic continuous-flow hydrogenation processes for the formation of vitamin and drugs precursors

**Anna Śrębowata<sup>1</sup>, Bartosz Zawadzki<sup>1</sup>, Rahma Abid<sup>1</sup>, Mirosław Krawczyk<sup>1</sup>, Krzysztof Matus<sup>2</sup> and Wioletta Raróg – Pilecka<sup>3</sup>**

<sup>1</sup>Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

<sup>2</sup>Materials Research Laboratory, Silesian University of Technology, Gliwice, Poland

<sup>3</sup>Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland

Catalysis research focuses on achieving 100% selectivity for the desired product. It is essential in the synthesis of fine chemicals, medicines and vitamins. This principle shall also apply to catalytic hydrogenation, a very important methodology in synthetic chemistry, of high relevance to manufacturing many fine chemicals, including pharmaceutical intermediates. Hydrogenations are usually carried out under batch conditions using noble metals such as Pd, Pt, Rh, and Ru as catalysts. Although they are very active in the hydrogenation process, their high cost and their inefficiency in the semi-hydrogenation of C≡C bonds or the chemoselective hydrogenation of C=C or C=O in the substrate, which contains two or more hydrogenable functionalities, intensified the research devoted in finding alternative catalysts containing lower amounts or deprived of noble metals. An attractive alternative for noble metals is readily available 3d transition metals, but they

usually require higher hydrogen pressure and temperature to attain comparable performance to noble metals. However, the use of the continuous-flow method significantly improves their catalytic properties. Therefore our research strategy focuses on developing nanocatalysts containing Ni, Co, Cu, and Fe - active in the liquid phase continuous-flow hydrogenations. In our studies, the continuous-flow mode was successfully implemented, e.g. for semi-hydrogenation of 2-methyl-3-butyn-2-ol and 2-butyne-1,4-diol towards forming essential A, E and B6 vitamins intermediates, several insecticides and antitumoral chemicals, and chemoselective hydrogenation of 2-methyl-2-pentenal towards 2-methylpentanal - an important intermediate for dyes, resins and drugs.

**Acknowledgements:** This work was supported by the National Science Centre in Poland within the project OPUS 17 UMO-2019/33/B/ST5/01271.

### Biography

Anna Śrębowata PhD DSc is the scientist at the Institute of Physical Chemistry, Polish Academy of Sciences in Warsaw. Currently, her research efforts are focused on the application of modern nanomaterials based on transition metals as catalysts for the continuous - flow hydrogenation processes of industrial and environmental importance. She is a co-author of over 50 original peer-reviewed papers published in the reputable international journals. Anna Śrębowata is a Member of the Polish Chemical Society, the Club of the Foundation for Polish Science Scholars, the Polish Zeolite Association and the Polish Club of Catalysis. In private life she is married with three children. She enjoys dancing and cooking.

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## Metal nanoparticles in the hydrogenation reactions in water

**Lucia Tonucci, Andrea Mascitti, Francesca Coccia and Nicola d'Alessandro**

*Università degli Studi "G. d'Annunzio" di Chieti-Pescara, Italy*

Lignin is an abundant waste-biomass, often used as a source of thermal energy; its aromatic nature makes it a resource for chemicals, innovative products, and alternative fuels [1]. The future development of the green industry is linked also to the valorization of this underutilized polymer. Recently, we prepared several metal nanoparticles (NPs) in aqueous solutions, using lignin as stabilizer, and we tested them as catalysts in several reactions of oxidation, reduction, cross-coupling, reaching excellent yields and selectivities [2]. In this work, we presented the preparation and characterization of the Pd, Pt, Ru, and Rh NPs. Pd NPs were larger (21 nm) and spherical in shape; Pt NPs were irregular; Ru and Rh NPs were smallest (1.9 and 5.3 nm, respectively). These metal NPs were used as catalysts in hydrogenation reactions of dicarboxylic acids in water at room pressure and temperature. The NPs catalyzed the selective transformation of fumaric and malonic acids to succinic acid, although with different yields: the best results were obtained in presence of Pd

and Rh NPs (80 and 100%). Carrying out the hydrogenations on muconic acids (also deriving from biomass), the formation of adipic acid, a key building-block in the polymer industry, was observed with all NPs but the full selectivity with Rh NPs was remarkable considering the mild conditions [3].

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3. L. Tonucci, A. Mascitti, A.M. Ferretti, F. Coccia, N. d'Alessandro, *Catalysts* 2022, 12, 1206.

### Biography

Lucia Tonucci is Assistant Professor of Inorganic Chemistry at "G. d'Annunzio" University of Chieti-Pescara (Italy). She graduated in Chemistry at University of Bologna and she completed her PhD at "G. d'Annunzio" University. Her research is focused on the Green Chemistry and the valorization of agro-industrial waste by catalysts (e.g., new metal nanoparticles) for chemistry and energy sectors.

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## Pd and Rh supported on ovine wool for catalytic reductions in batch and in flow mode

**Francesca Coccia, Lucia Tonucci and Nicola d'Alessandro**

*Università degli Studi "G. d'Annunzio" di Chieti-Pescara, Italy*

**H**eterogeneous catalyst is an attractive form of catalyst from an industrial point of view, since it guarantees its reuse for several times and avoids purification steps not causing the leaching in the reaction mixture. Textile industry offers an emerging support for catalyst such as wool or cotton fibers; in particular wool, as a recovery material, with its amino-acid structure allows different attach protocols for many kinds of molecules<sup>1</sup>. We propose an easy synthesis of Pd and Rh nanoparticles (NPs) on ovine wool in water. We have tested their catalytic activity in reduction reaction of maleic acid to succinic acid

and of p-nitrophenol to aminophenol in water under H<sub>2</sub> flow or using a chemical reducing agent. Chemical and morphological characterization of NPs was studied by TEM, ATR, XRD. Changes in morphology of NPs are evident if modified wool are used as active support for NPs formation. Experiments of reduction in flow mode with a chemical reducing agent were tested using as catalytic reactor an old HPLC column home packed with metal NPs functionalized wool.

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### Biography

Francesca Coccia is a researcher of Inorganic Chemistry at "G. d'Annunzio" University of Chieti-Pescara (Italy). She graduated in Pharmaceutical Chemistry at University of Chieti and she completed her PhD in Inorganic Chemistry at "G. d'Annunzio" University. She continued her research at the University of Milan and at CNR of Milan. Her research is focused on the Green Chemistry, the valorization of agro-industrial waste by catalysts and functionalization of different materials..

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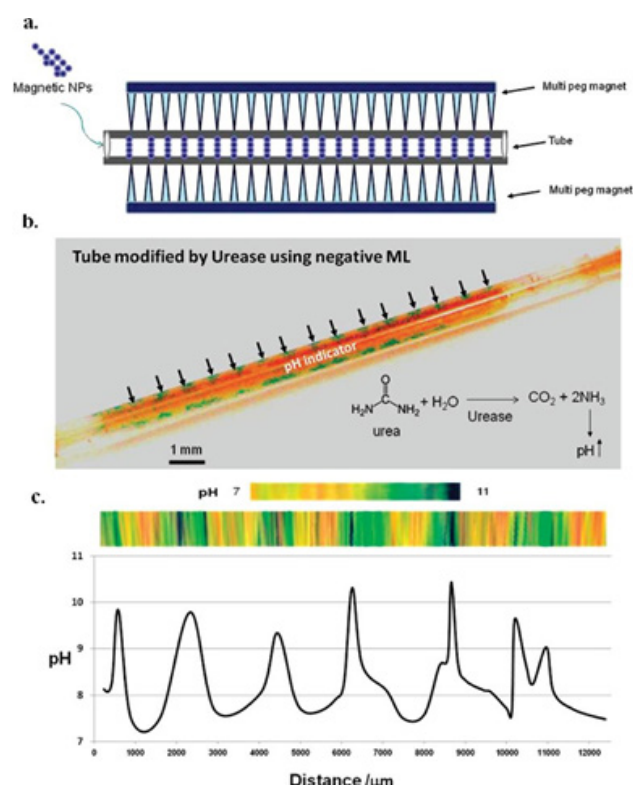
## Producing Portable Microreactors into Closed Volume

**Amos Bardea**

*Holon Institute of Technology (HIT), Holon, Israel*

The new surface patterning method is based on Magneto Lithography (ML). ML is a “bottom-up” method, but at the same time, it provides desired high throughput capabilities for mass production. It is based on applying a magnetic field on the substrate using paramagnetic metal masks that define the spatial distribution and shape of the applied field. The second component in ML is ferromagnetic nanoparticles (NPs) that are assembled onto the substrate according to the field induced by the mask. ML can be used for applying either a positive or negative approach. In the positive approach, the magnetic NPs react chemically with the substrate. Hence, the magnetic NPs are immobilized on selective locations, where the mask induces a magnetic field, resulting in patterned substrates. In the negative approach, the magnetic NPs are inerted into the substrate. Hence, once they pattern the substrate, they block their binding site on the substrate from reacting with another reacting agent. After the adsorption of the reacting agent, the NPs are removed, resulting in a negatively patterned. ML does not depend on the surface topography and planarity, and can pattern non-flat surfaces and the inside surfaces of a closed volume, therefore, ML allows the chemical patterning of the inside of tubes. The ML can pattern the inside of tubes by applying either positive or negative routes. The ability to pattern tubes opens up new dimensions in sensors development and applications. Here

we demonstrated the ability to pattern the inner surface of a tube with relatively small molecules. However, for sequential processes, the reaction between the reactant in the solution and the one adsorbed on the surface must be localized. Next, we will demonstrate the ability to pattern the inner part of the tube with enzyme and reveal the localization of the reaction. Here, the enzyme was patterned on the inside of the 500  $\mu\text{m}$  diameter tube at different places using the negative ML approach.



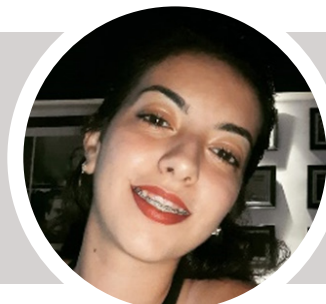
## Biography

Dr. Amos Bardea is senior lecturer and head of the undergraduate program at the faculty of engineering at Holon Institute of Technology (HIT). He got in 2000 his Ph.D. from Hebrew University of Jerusalem for his thesis on developing high sensitivity electronic sensors.

After graduating, he worked at Intel for several years as a senior engineer and led implementation of advanced technologies of micro and nano processors in manufacturing. In 2007 he joined to Department of Chemical Physics at the Weizmann Institute of Science. He developed a novel method for nano and molecular patterning by applying magnetic fields, know "Magnetolithography" and applied the new method for developing ultra-sensitive DNA and RNA sensors based on microfluidics and molecular Photonics.

In 2011 Dr. Bardea joined to the Faculty of Engineering at HIT. He is pioneers in teaching nanotechnology in higher education. He developed the first course in 2005 since he teaches graduate students at Bar-Ilan Institute of Nanotechnology & Advanced Materials (BINA) and at the faculty of engineering in HIT. Amos Dr. Bardea hold B. A graduate in Philosophy from Bar-Ilan University and Sciences Teaching Certification from Weizmann Institute of Science.

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## Characterization and application of hybrid synthesized by sol-gel method

**Dehhaoui salma, Jermoumi touriya, Shaim abdelillah,  
Rair driss and Chahine abdelkrim**

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The aim of the study was to synthesize a hybrid performed by sol-gel process in order to mix properties of organic and inorganic compounds that received a lot of attention in recent decades for their versatile applications. The Benzimidazol-doped  $\text{TiO}_2$ - $\text{P}_2\text{O}_5$  composite was evaluated as a good catalyst.

The obtained hybrid have been characterized using Scanning Electron Microscope (SEM), Energy Dispersive X-Ray Analysis (EDX), thermogravimetric analysis (TGA) coupled with differential thermal calorimetry (DTA) and Fourier

Transform Infrared (FTIR) spectroscopy.

Each of these techniques allowed us to understand the physico-chemical behavior of the composite.

X-ray diffraction confirmed the totally amorphous structure, the infrared spectroscopy show the different links of the composition, SEM results presented the hybrid morphology, The EDX data allowed to know the quantitative percentage of the elements present on samples, DTA/TGA resume the evolution of the hybrid under temperature effect.

### Biography

Dehhaoui salma started her PhD in 2022, In the Laboratory of Advanced Materials and Process Engineering, Faculty of Science, Ibn Tofail University under the supervision of Pr. Chahine Abdelkrim

Her studies are focused on the properties of phosphate-based materials, for the purpose of optimizing and getting a variety of applications..

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## Development of a novel glasses based on phosphate and its application as a promising adsorbent for crystal violet dye removal

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The present study is about the use of glasses all by themselves and for the first time as adsorbents to improve their adsorption capacity for the removal of crystal violet dye from aqueous solutions. New samples of glasses based on phosphate were synthesized using conventional melt quenching method and characterized by X-Ray analysis, which confirms the amorphous structure of our samples, Fourier Transform Infrared (FT-IR) shows that V2O5 behaves as a network former at high concentrations, density and molar volume indicates the formation of new interconnections and destabilization in the structure of our glasses. Confirming the IR spectroscopy results as a function of V2O5 content. The glasses based on phosphate were efficiently employed for the first time as an adsorbent crystal violet (CV) dyestuff from water. These glasses showed an interesting capacity to absorb the

crystal violet dye by a removal efficiency of about 98% after 1h of stirring. The CV dye adsorption performance was investigated as a function of several operating conditions. Isothermal and kinetic adsorption modeling indicates a good fit between the Langmuir isotherm and pseudo-second order models. Kinetic approach studies for crystal violet dye removal clearly indicated that the results of the adsorption process followed the pseudo second order and Langmuir models. From a thermodynamic point of view, the CV adsorption process occurred spontaneously and exothermically. These findings revealed that the synthesized glasses based on phosphate exhibited a high potential for wastewater treatment containing CV.

**Keywords:** Glasses; phosphate; surface chemistry; Cristal violet; Adsorption.

### Biography

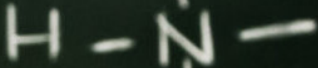
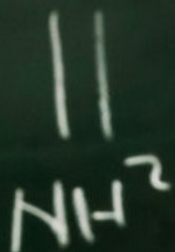
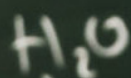
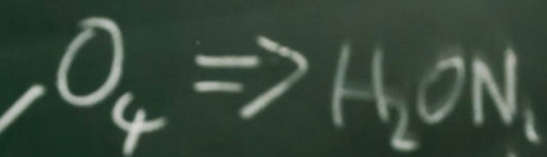
Dehhaoui salma started her PhD in 2022, In the Laboratory of Advanced Materials and Process Engineering, Faculty of Science, Ibn Tofail University under the supervision of Pr. Chahine Abdelkrim-

Her studies are focused on the properties of phosphate-based materials, for the purpose of optimizing and getting a variety of applications.

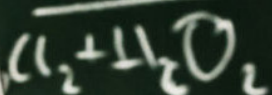
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## Demonstration of syngas production process directly using low-concentration CO<sub>2</sub> from process exhaust gas

**Hyun-Ji Kim<sup>1</sup>, Tae-Jin Kang<sup>1</sup>, Ji-Hyeon Kim<sup>1</sup>, Jin-Ho Kim<sup>1</sup>, Hyo-Sik Kim<sup>1</sup>, Jae-Hong Ryu<sup>1</sup>, Suk-Hwan Kang<sup>1+</sup>, Ye-Ji Lee<sup>2</sup> and Soo-Chool Lee<sup>2</sup>**

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Climate change due to greenhouse gases is emerging as a global issue, and we are trying to suppress the global average temperature by introducing systems such as CBAM(Carbon Bord Adjustment Mechanism) and ETS(Emission Trading Scheme) worldwide. In order to achieve the goal of carbon reduction, CCU(Carbon Capture Utilization) technology, which captures CO<sub>2</sub> from process exhaust gas or utilizes CO<sub>2</sub> to produce syngas for fuel, is attracting attention. Dry reforming technology, which is one of the conversion technologies using a catalyst to utilize CO<sub>2</sub> as a material with high added value, is of interest from researchers because it uses greenhouse gases(CO<sub>2</sub> and CH<sub>4</sub>) to produce synthesis gas (CO and H<sub>2</sub>). However, the DRM(Dry reforming of methane) requires a lot of energy because it includes a capture

process to use the high concentration of CO<sub>2</sub> emitted from the process, resulting in additional CO<sub>2</sub> emission. In addition, since the DRM is a strong endothermic reaction, the temperature of the catalyst is lowered during the reaction, causing problems such as coke generation, catalyst deactivation, and reactor blocking etc. In this study, to solve the problems of the DRM, an dry autothermal reforming process(DARM) that produces syngas by directly reacting low concentration CO<sub>2</sub> in the flue gas with bio-CH<sub>4</sub> without a separate carbon capture utility was developed. Thus, the characteristics of DARM will be described in comparison with DRM.

**Funding:** This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (Project No. NRF-2022M3J2A1053003).

### Biography

Received a master's degree in chemical engineering from Kyungpook National University in 2019. Worked as a researcher at the KEPRI from 2019 to 2020. Working at IAE since 2021.

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## A study on dry reforming reaction on Ni-based catalyst for direct utilization of exhaust gas

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Due to global warming caused by greenhouse gases, reduction of greenhouse gases has become an important issue worldwide. The IEA(International Energy Agency) has announced a plan for the realization of carbon neutrality and net-zero in 2050. CCUS (Carbon Capture Utilization and Storage) was mentioned as a key technology for CO<sub>2</sub> capture and carbon neutrality at the same time as CO<sub>2</sub> emission reduction in various fields such as energy, industry, and transportation. The CCUS technology has been proposed as a solution in the hard to abate field, and is attracting a lot of attention in that it can recycle carbon dioxide, which accounts for the largest proportion of greenhouse gases, into useful materials. Among various methods for utilizing greenhouse gases,

the greenhouse gas conversion method using a catalyst is typically divided into DRM (Dry Reforming of Methane) and DARM (Dry Auto-thermal Reforming of Methane). DRM and DARM using a Ni-based catalyst were compared that the thermodynamic conversion, the composition of the product gas according to the CO<sub>2</sub>/CH<sub>4</sub> ratio, the coke production amount, the catalyst activity, and the reaction characteristics of the catalyst according to the temperature. In this study, based on the above characteristics, the catalyst and process conditions for directly utilizing the process exhaust gas were considered.

**Acknowledgement:** This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (Project No. NRF-2022M3J2A1053003).

### Biography

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## Biological-photocatalytic ( $\text{TiO}_2/\text{Na}_2\text{S}_2\text{O}_8/\text{solar}$ ) coupled pilot plant for wastewater detoxification (pharmaceuticals and pesticides) and its reuse for tomato crop irrigation

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In Mediterranean countries, water scarcity has caused the necessity of reuse reclaimed waters as an essential practice for crop irrigation. The occurrence of emerging pollutants (EPs) in wastewater may represent a risk for human health and environment owing to their release in soil and translocation to plants. This work focuses on the detoxification of wastewater polluted with 2 pharmaceuticals (clarithromycin and venlafaxine) and 2 pesticides (imidacloprid and thiachloprid) using a coupled biological-photocatalytic facility under natural sunlight for tomato irrigation under agricultural field conditions in Murcia (SE of Spain). The photocatalytic process was done using the tandem  $\text{TiO}_2/\text{Na}_2\text{S}_2\text{O}_8$  under natural solar radiation.  $\text{TiO}_2$  P25 Degussa was used as photocatalyst due to its convenient advantages. EPs residues were extracted from water, soil and tomato samples and were analyzed by HPLC/MS2 (QqQ). Almost complete disappearance of EPs

residues was achieved after coupled biological (from 56% for clarithromycin to 91 % for venlafaxine) and photocatalytic (> 98 % for 4 EPs) treatments at pilot plant. Field experiments were conducted using different irrigation supplies: contaminated water, uncontaminated water, and reclaimed wastewater (RWW). The impact of using RWW on the quality of tomatoes grown was also assessed (total yield and quality parameters). Therefore, solar heterogeneous photocatalysis, with  $\text{TiO}_2$  as photocatalyst, is presented as a promising technology to be incorporated as a tertiary process in wastewater treatment plants

**Acknowledgments:** Ministry of Science and Innovation (Project PID2019-106648RB-I00/AEI/10.13039/501100011033) and technical assistance from H. Jiménez, J. Cava, I. Garrido, M.V. Molina, E. Molina, I. Fernández, C. Colomer and J.L. Lozano.

### Biography

He obtained his degree in Chemistry (1997) and Ph.D. in Chemistry (2001) at University of Murcia. Postdoctoral stay at the Université Libre de Bruxelles. After this period, he worked as Head of I+D Area in the Chemical Microbiological Laboratory, deepening his knowledge in the development of new methodologies for pesticides analysis and other substances of environmental interest. Since 2003 he is a researcher at Instituto Murciano de Investigación y Desarrollo Agrario y Medioambiental. His activity focuses on the area of environmental chemistry and development/application of technologies for water/soil decontamination. He has participated in 20 national and 4 international projects. Contributions: >135 articles (h: 29), > 100 scientific communications. Supervision of 7 PhD dissertation, 11 Bachelor's Thesis and 2 MSc Thesis.

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## Chemiresistive polymer percolation network gas sensor created with a nanosphere template

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Developing chemiresistors based on conducting polymer (CP) is regarded as one of the simplest ways of gas sensing. To improve the device sensitivity and limit of detection (LOD), various approaches have to date been developed. Among all the reported approaches, nanostructuring is regarded as an effective strategy owing to desirable morphologies with higher surface-to-volume ratios. Recently, electrical percolation has been reported as another effective approach to improve sensing performance since a small number of interactions between the analyte molecules and the CP percolation network can lead to a relatively large resistance change. Therefore, it is a natural step to combine these promising approaches for further investigation and device improvement. Here, electrochemical polymerisation to create percolation networks is coupled with nanosphere templating to facilitate

nanostructuring. We have created nanostructured polypyrrole (PPy) chemiresistive sensors for ammonia detection with the aid of a nanosphere template. Polystyrene (PS) nanospheres are deposited on interdigitated electrodes to form a template, and chronoamperometry is then used to grow PPy between the electrodes within the gaps of the nanospheres. The PPy growth is controlled to create electrical percolation networks. After removal of the nanospheres, the percolation behaviour and sensing response of the nanostructured PPy sensors are investigated. The nanostructured sensors show higher sensitivity and lower LOD to ammonia than percolation networks prepared without nanosphere templates. An optimal nanostructured ammonia percolation sensor with a chemiresistive sensitivity of  $2.59 \pm 0.20$  % ppm<sup>-1</sup> and a LOD of  $71 \pm 6$  ppb is obtained.

### Biography

Weishuo Li received his B.Sc degree in Macromolecular Materials and Engineering in 2015 from Beijing Institute of Technology and M.Sc. degree in Advanced Materials and Mechanics in 2018 from Peking University. Supervised by Prof. Hong Meng during his master career, he received comprehensive academic training in the field of organic electronics, spanning from the synthesis and characterization of conjugated polymers and metal organic frameworks to their application in supercapacitors and electrochromism. Now he is a PhD student in materials supervised by Prof. Martin R. Castell at the University of Oxford. He is carrying out research into conducting polymer gas sensors.

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## Numerical simulations to support the development of magnetized gears

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The work here presented had as main objective the production of injection molded gears that are magnetized during the developed manufacturing process. Through this process, it is possible to produce the magnetized gears in one sole process, that combines the manufacturing process of Powder Injection Molding and the process of magnetizing the produced gears. This is done by subjecting the produced parts to high intensity magnetic fields, which is typically done separately, having higher cycle times and costs. For this, a material comprised of metal (Strontium Ferrite) and polymer (Polyamide / Nylon 12) was used to produce these gears. The metal is the main material, being responsible for magnetization, and the polymer is added to increase the processability and fluency of the metal. To assist in the development of this magnetized gears, a numerical methodology was used to analyze the mechanical behavior of both the final product and a thin injection mold plate. The numerical simulations of the

thin mold plate allowed analyzing its structural integrity and assure that it would withstand the applied loads during the injection process, as well as analyzing its thickness and material to be used for the production of the mold, allowing the selection of the configuration that led to a lower deformation. The numerical simulation of the final product, aimed to analyze the effect of a possible weak homogenization of metal particles on the gear's teeth. This aimed to evaluate the feasibility of this concept regarding its mechanical behavior, which might be influenced by the metal distribution throughout the part, since if it is not uniform may cause the weakening of some areas.

The Magnetized Gears project consortium is constituted by GLN Molds, the promoting company, and GLN Plast, CeNTI, PIEP and the University of Minho as co-promoters. The project is co-financed by Portugal 2020, under the Operational Programme for Competitiveness and Internationalization (COMPETE 2020), from European Regional Development Fund (ERDF).

### Biography

Lourenço Bastos has a Master's Degree in Polymer Engineering (2015) from the University of Minho, Portugal, with a specialization in material science, material modelling, polymer processing and numerical simulation. He has since worked as a researcher in the field of Computer Aided Engineering. Currently, he is a research and development engineer at PIEP - Centre for Innovation in Polymer Engineering. His research activities are mainly focused on numerical simulations, including CFD, structural and fluid-structure interaction using commercial software. He has participated in several research and development projects in different areas of expertise, including automotive, medical, railway, civil, and others.

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## Dielectric/Electronic ink study for electronic circuit combination

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In-mould electronics (IME) technology integrates films with printed electronics into the injection moulding process, to produce functional 3D plastic parts. By combining printed functional circuits with the injected component, the post-process of assembly and the need for mechanical buttons are eliminated, translating into a reduction of supplementary electronic components. In the first step of IME, the film is printed with different layers - conductive inks and insulation layers. In this study two different printed circuits were overlaid in order to evaluate the possibility of having different functionalities in the same area (capacity sensors with different ends), diminishing the necessary printed area in the moulded component, leading to the possibility of reducing the dimensions of the final component. A sandwich structure was tested (conductive silver ink circuit – dielectric ink – conductive silver ink circuit) in order to evaluate the insulation capability of the dielectric

ink and the functionality of the two different silver ink printed circuits. For the substrate, films of Polycarbonate (PC) were used. The number of printing layers for the dielectric ink influence was studied on the circuit functionality. The resulting printed films were analysed by scanning electron microscope (SEM) in order to evaluate ink miscibility and silver ink migration. Throughout the study, the circuit functionality was tested.

The project consortium is composed of Fehst Componentes, the promoting company, PIEP - Innovation in Polymer Engineering, and the University of Minho. This work was supported by the European Regional Development Fund (ERDF), through the Competitiveness and Internationalization Operational Program (COMPETE 2020) of the Portugal 2020 Program [FEHST AVANTGARDE INTERIORS POCI-01-0247-FEDER-072283].

### Biography

Cátia Araújo has a Master's Degree in Polymer Engineering from the University of Minho, Portugal. She has since worked as a researcher in the field of injection moulding process (thermoplastic polymers). She is currently working at PIEP - Centre for Innovation in Polymer Engineering, in advanced manufacturing processes (thermoplastics). Her research interests and experience are focused on Injection Moulding Process Simulation (conventional and non-conventional), In-Mould Decoration (IMD, IML, IME), Insert Moulding, Foam Injection Moulding, In-cavity Sensorying, and Monitoring and Material Characterization.

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## An experimental study of the effect on mechanical properties of virgin and recycled high-density Polyethylene blends

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The development of value-added products made from post-consumer recycled plastic is becoming increasingly important to a more sustainable society. In order to achieve this goal, recycling studies of these plastics are more and more necessary, since their use generally affect the mechanical properties and therefore the quality of the end products.

This study aims to determine the effect on mechanical properties of virgin high-density polyethylene (v-HDPE) and recycled high-density polyethylene (r-HDPE) blends and assess the possible end substitution of 100% v-HDPE for 100% r-HDPE. Mechanical tests were performed on different blending ratios of HDPE from 100% v-HDPE up to 100% r-HDPE.

This study reveals that the r-HDPE was successfully extruded. The mechanical properties of v-HDPE/r-HDPE blends over the complete concentration range were thoroughly

investigated in this work. Tensile properties, elongation and modulus of elasticity were analyzed for blends with 60, 70, 80 and 100% r-HDPE. With regard to the modulus of elasticity, the blend with 30% v-HDPE and 70% r-HDPE presented a value of  $1070 \pm 89$  MPa, equivalent to the modulus of 100% v-HDPE ( $1069 \pm 89$  MPa). Furthermore, it was observed a tiny reduction of 2% in the 100% r-HDPE modulus comparing to the 100% v-HDPE value. However, it was found that tensile properties for r-HDPE shown a tensile strength reduction of 20% comparing to the reference values of v-HDPE.

In general, it can be concluded that the mechanical properties of r-HDPE are closer to the v-HDPE, and they have huge potential for plastic recycling.

Project 46091 – Better Plastics, financed by Portugal 2020 and European Union, through the European Regional Development Fund (ERDF).

### Biography

Sónia Miranda has a Master's Degree in Polymer Engineering from the University of Minho, Portugal. She currently works at PIEP - Innovation in Polymer Engineering Center, where she has gained extensive experience in extrusion, compounding and advanced materials. Her expertise includes working with a diverse range of polymer materials, including natural polymers and high-performance polymers. Her specialization is in the development of new thermoplastic-based materials through extrusion and composition technologies.

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## A study on carbon vs silver inks conductivity resistance in In- Mould Electronics (IME) process

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In-Mould Electronics (IME) is a technology in which electronic components are introduced in the injection moulding (IM) cavity and over-moulded with melted polymer. This technology has been widely embraced by several industries with particularly high demand in the automotive industry where it is possible to produce lighter components with fewer steps but with high aesthetic standards. However, the IME technology possesses some degree of complexity due to the high temperatures exerted during IM process, originating ink washout, and consequential loss of functionality of the component. The high prices applied in the process due mainly to the price of the silver-based ink pushed for an alternative. Carbon-based inks have for a long time been used in IME due to lower prices and higher thermal resistance, making them more suitable for the IM process however, they possess lower conductivity. As the IM process is known for high shear rates and high melt temperature, during the process the imprinted ink is washed by the polymer melt. Therefore, the evaluation of the resistance to wash-out of carbon

vs silver-based inks is an important assessment for the manufacturing industry. In this study, carbon ink appropriate for the IME process was printed in a Polycarbonate (PC) substrate. The samples were thoroughly characterized through a scanning electron microscope (SEM) and the resistivity of the samples was measured at every step. Additionally, in the IM phase, process conditions were analysed through a design of experiments (DOE) to evaluate which parameter could have the most influence on washing the ink. The obtained results with carbon-based ink were compared with silver-based ink in the IME process.

The project consortium is composed of Fehst Components, the promoting company, PIEP -Innovation in Polymer Engineering, and the University of Minho. This work was supported by the European Regional Development Fund (ERDF), through the Competitiveness and Internationalization Operational Program (COMPETE 2020) of the Portugal 2020 Program [FEHST AVANTGARDE INTERIORS POCI-01-0247-FEDER-072283].

### Biography

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## Powder Injection Molding simulation to study the influence of flow behaviour of highly filled materials with magnetic particles for automotive application

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Powder Injection Moulding (PIM) is a process that can be used for the production of magnetic components by injecting a polymer-bonded magnetic compound with filler contents between 55 and 65 vol%. These composite materials comprise hard magnetic particles, namely ferrite, and rare-earth materials embedded in a polymer binder matrix. The large concentration of metallic particles leads to a viscosity increase of the composite material, which can lead to several problems during the filling phase of the process. This work aims to investigate an injection mould with an integrated magnetization system, allowing the magnetization of the parts in the mould during the injection process. This production approach leads to the elimination of additional post-processing magnetization procedures, enabling a reduction of the process cycle time and cost, and an increase of the manufacturing efficiency. To support the development of this injection mould, numerical simulations based on the software Moldex3D PIM have been performed to analyse the flow behavior of the composite material. As the powder binder phase separation (black

lines) can compromise the surface finish and the mechanical performance of the component, the particle concentration distribution throughout the entire part has been analysed. The results obtained in this simulation have been integrated into another study that analysed the mechanical performance of both part and mould, using structural simulations. This work also includes gating and cooling system analyses since both have an impact on product quality and productivity. In addition, as permanent magnets are incorporated into the injection mould, they are subjected to high temperatures. To analyse if their magnetic characteristics can be compromised, a numerical analysis of temperature has also been performed.

The Magnetized Gears project consortium is constituted by GLN Molds, the promoting company, and GLN Plast, CeNTI, PIEP and the University of Minho as co-promoters. The project is co-financed by Portugal 2020, under the Operational Programme for Competitiveness and Internationalization (COMPETE 2020), from European Regional Development Fund (ERDF).

### Biography

Rita Marques received her Master's Degree in Polymer Engineering from the University of Minho, Portugal, in 2016. She has worked as a research engineer with expertise in the simulation of conventional and non-conventional injection molding. She was actively involved in numerous research and development projects for several sectors, including automotive and medical. Her research activities were mainly focused on numerical simulations, using commercial software. Currently, she is a project manager in the group Advanced Manufacturing Processes (Polymers) at PIEP - Centre for Innovation in Polymer Engineering.

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