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ABSTRACT BOOK

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DAY-1, JUNE 29, 2026

Plenary Talks

Catalysis for Bio-Chemicals and Bio-Fuels: Scientific and Technical Achievements in an Evolving Landscape

Fabrizio Cavani*

Alma Mater Studiorum Università di Bologna, Dipartimento di Chimica Industriale "Toso Montanari", Bologna, Italy

Abstract:

In recent years, the biorefinery concept has evolved from a facility primarily focused on biofuels to an integrated multi-product system, oriented towards zero-waste operations and the principles of the circular bioeconomy. This is not only a shift from the processing of "first-generation" food crops to advanced second- and third-generation feedstocks for the production of high-value chemicals along with energy, but also is driven by a growing interest in unconventional waste streams, such as municipal organic waste, agricultural residues, oilseed cakes and seaweed; and a particular focus on lignin depolymerization and CO_2 valorization. Industrial strategies also include process intensification and digitalization, the retrofitting of fossil-fuel refineries for biomass management, and the development of new advanced tools for sustainability assessment. Catalysis has played and continues to play a key role in facilitating this evolving landscape. The design of new multifunctional systems aims to enable, for example, the development of one-pot processes for biomass and waste valorization and of photocatalytic and electrocatalytic new technologies, and the integration of green-H_2 into existing industrial hydrogenation processes. This presentation will illustrate some examples of novel catalytic systems developed in our laboratory over the last decade, which illustrate the evolving goals of biorefineries.

Biography:

Fabrizio Cavani received his PhD in Industrial Chemistry in 1986. After 4 years spent in EniChem Synthesis, he won the position of assistant professor at the University of Bologna, where he is currently full professor of Industrial Chemistry.

Emerging Catalysis Process for Effective Energy Storage

Qiang Zhang, Tsinghua University, China

Colloidal Metal Nanocrystals as the Next-Generation Catalytic Materials

Younan Xia*

Department of Materials Science and Engineering, Department of Biomedical Engineering, Johns Hopkins University, Baltimore, Maryland 21218, USA

Abstract:

Heterogeneous catalysis is of critical importance to the world's economy as it is involved in more than 90% of the chemical processes. Among various catalytic materials, metals easily stand out because of their ability to donate and accept electrons for catalyzing both reduction and oxidation reactions, as well as the capability to adopt different oxidation states depending on the reaction environment. Heterogeneous catalysts based on metals are indispensable for the production of numerous industrial chemicals and pharmaceuticals. Recent success in the synthesis of colloidal metal nanocrystals with controlled shapes offers many opportunities to not only maneuver their physicochemical properties but also optimize their figure of merits in a wide variety of applications. In particular, heterogeneous catalysis and surface science have benefited enormously from the availability of this new class of nanomaterials as the atomic structure presented on the surface of a nanocrystal is ultimately determined by its geometric shape. The immediate advantages may include significant enhancement in catalytic activity and/or selectivity and substantial reduction in materials cost while providing a well-defined model system for mechanistic study. With a focus on the monometallic system, I aim to provide a comprehensive account of recent progress in the development of colloidal metal nanocrystals with controlled shapes, in addition to their remarkable performance in a large number of catalytic and electrocatalytic reactions. It is hoped that this talk offers the impetus and roadmap for the development of next-generation catalysts vital to a broad range of industrial applications.

Biography:

Dr. Younan Xia is a Bloomberg Distinguished Professor at Johns Hopkins University, with joint appointments in Department of Materials Science and Engineering and Department of Biomedical Engineering. He received a B.S. degree in chemical physics from the University of Science and Technology of China (USTC) in 1987, M.S. degree in chemistry from University of Pennsylvania (with Alan G. MacDiarmid) in 1993, and Ph.D. degree in physical chemistry from Harvard University (with George M. Whitesides) in 1996. His group invented numerous nanomaterials with well-controlled properties for use in applications related to plasmonics, electronics, display, catalysis, energy conversion, controlled release, drug delivery, nanomedicine, and regenerative medicine. Notably, the silver nanowires invented by his

group were commercialized for the manufacturing of flexible, transparent, and conductive coatings key to applications such as touchscreen display, flexible electronics, and photovoltaics. His technology on the alignment of electrospun nanofibers was commercially used for multiple clinical products in regenerative medicine, including those for the management of surgical and trauma wounds. Xia has co-authored over 900 publications in peer-reviewed journals, together with a total citation of more than 220,000 and an h-index of 224. He has been named a Top 10 Chemist and Materials Scientist based on the citation data. He has received many prestigious awards, including the Linus Pauling Medal (2024), ACS Award for Creative Invention (2023), MRS Medal (2017), ACS Award in the Chemistry of Materials (2013), NIH Director's Pioneer Award (2006), and NSF CAREER Award (2000). More information can be found at http://www.nanocages.com

Photocatalytic Water Splitting to Produce Green Hydrogen and Related Fuels [Online]

Kazunari Domen[1,2*]

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[2] *Office of University Professors, The University of Tokyo, Japan*

Abstract:

The large-scale production of low-cost green hydrogen and related fuels is critically important for society today and in the future. At present, the most practical route to chemical energy production is water electrolysis powered by renewable electricity from wind and photovoltaics (PV). However, it has become increasingly clear that hydrogen produced via this pathway remains expensive. Although hydrogen production using water-splitting photocatalysts is still at the research and development stage, it offers the potential for scalable, low-cost hydrogen generation in the future. Realizing this potential requires the development of water-splitting photocatalysts with high solar-to-hydrogen conversion efficiency. In this lecture, several representative water-splitting photocatalysts are introduced, with a focus on their structures and reaction mechanisms. Key challenges in developing practical photocatalysts with high solar energy conversion efficiency for real-world deployment are also discussed. As one strategy for large-area implementation, the lecture presents the current status of photocatalyst sheets and water-splitting panels under development by the authors. In addition, the lecture reviews the state of the art in safely separating hydrogen from the hydrogen–oxygen mixtures generated by photocatalytic water splitting. Finally, while storage and transportation of the produced green hydrogen remain important issues, the lecture also considers several routes for converting it into green fuels through DSS operation.

Biography:

Kazunari Domen is a University Professor at The University of Tokyo and a Distinguished Professor at Shinshu University. He received a B.Sc. (1976) and Ph.D. (1982) in chemistry from the University of Tokyo. He joined Tokyo Tech and was promoted to a professor in 1996. He moved to the University of Tokyo in 2004 and was appointed to a University Professor in 2019. He was cross appointed as a Special Contracted Professor at Shinshu University in 2017 and Distinguished University Professor in 2025. His research focuses on the phphotocatalystsevices for efficient solar hydrogen generation via water splitting.

Green Shades in Catalysis for Fine Chemicals and Pharmaceuticals

Luigi Vaccaro*

Laboratory of Green S.O.C. – Dipartimento di Chimica, biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, Perugia 06123, Italy

Abstract:

Our approach to modern green chemistry is focused on the general idea that green/efficient processes are those designed to minimize waste by the rational combination of different technologies and the use of specific metrics needed to quantify the advance in terms of sustainability.

Our research program is mainly committed to the definition of efficient and sustainable synthetic tools by combining the development of several crucial areas of investigation:

i) use of safer reaction media,

ii) ii) preparation and use of nanostructured heterogeneous and reusable catalytic systems;

iii) iii) definition of continuous-flow reactors allowing a minimal waste production and high productivity;

iv) iv) applications of metrics and LCA to assess the overall sustainability of the results.[1]

Among the different projects, we are currently dedicated attention to the valorisation of waste for the preparation of recoverable catalytic systems and electrodes to define efficient protocols based on the use of continuous-flow reactors and electrochemistry.

In this contribution it will be presented an overview of our vision and ongoing research in the field.

[1]Some recent examples L. Vaccaro et al: *ACS Catal.* **2025***, 15,* 7263−7282*; Green Ener. Environ.* **2025**, *10*, 733-755*; Chem. Eng. J.* **2025***, 504,* 158822; *Green Chem.*, **2025**, *27*,

633−641; *ACS Catal.* **2025**, *15*, 4, 3367–3376; *Green Chem.*, **2025**, *27*, 3869–3878; *ChemSusChem* **2025**, *18*, e202402011.

Biography:

Luigi Vaccaro is a Full Professor at the University of Perugia, where he is leading the Green S.O.C. group, http://greensoc.chm.unipg.it. He is Fellow of the Royal Society of Chemistry (FRSC) and he is currently appointed as Associate Editor of Green Chemistry (RSC) and of Beilstein Journal of Organic Chemistry. His recent recognitions comprise the Pino Medal from the Organic and Industrial Divisions of the Italian Chemical Society (2023) and the Rita Levi Montalcini award (2025). His research is aimed at developing different aspects of chemistry to define sustainable and optimized processes. Luigi has published ca. 320 scientific contributions with an H-index of 65, and about 32000 citations.

Keynote Talk

Where to Look for Shape Selectivity? The Strange Cases of Catalysis on Ferrierite

Francesco Di Renzo*, Jonathan Fabian Sierra-Cantor, Corine Gérardin, Nathalie Tanchoux

ICGM, University of Montpellier-CNRS-ENSCM, Montpellier, France

Abstract:

It is uncommon that a reaction mechanism has to be developed for the sites of a specific zeolite. This has occurred in several instances for the Brönsted acid sites of ferrierite, a zeolite with a bidimensional network of 10- and 8-member-ring micropores. Ferrierite is the industrial reference catalyst for butene isomerization since more than thirty years but its exceptional selectivity is remained unexplained until an extremely ingenious research work has elucidated a unique carbon-pool mechanism at the micropore mouth. In more recent years, all the resources of crystallography, spectroscopy and, above all theoretical chemistry, have been gathered to propose reasonable explanations of the unprecedented reverse selectivity in isobutanol dehydration to n-butene or of dimethylether carbonylation mechanism. The used methods and the obtained results can provide inspiration for mechanisms and processes in the whole field of nanostructured catalysts.

Biography:

After a degree in chemical engineering and a PhD in industrial chemistry from the Politecnico di Milano, Francesco DI RENZO moved to the CNRS, working on the elaboration of catalysts

for petrochemistry and the valorisation of renewables. Former president of the French Zeolite Group, he is now emeritus research director at the ICGM, Institut Charles Gerhardt in Montpellier. Jonathan Fabian SIERRA-CANTOR successfully completed at ICGM a PhD thesis on ferrierite catalysis for bioresources. Corine GERARDIN is head of the D3, Department of Hybrid and Porous Materials at the ICGM, where Nathalie TANCHOUX leads the catalysis team.

Invited Talks

Towards Accurate Modeling of Elementary Reaction Steps in Heterogeneous Catalysis via Insights from Gas-Surface Dynamics

Jörg Meyer*

Leiden Institute of Chemistry, Gorlaeus Laboratories, 2300 RA Leiden, The Netherlands

Abstract:

Advancements in quantum chemistry codes and, more recently, machine learning have significantly improved the modeling of gas-surface dynamics, enhancing both accuracy and complexity [1]. This progress has mainly focused on comparing simulations with molecular beam experiments. However, although dynamic catalysis is attracting increasing attention [2], decades-old static models still predominate in heterogeneous catalysis.

One notable example is the Fridman-Macheret (FM) α model, used to quantify increased turnover frequencies (TOFs) in plasma-assisted versus conventional (temperature-driven) heterogeneous catalysis, fostering hopes for a scalable and sustainable alternative. A key focus has been ammonia synthesis and vibrationally excited plasma states, as dissociative chemisorption of N_2 on metal catalysts is typically rate-limiting. Micro-kinetic modeling based on transition state theory (TST) requires extension with vibrational-state-dependent rate constants. Mehta et al. [3] proposed that the efficient TST+FM-α model used in gas-phase reactions can also describe vibrational effects on surface reactions.

In this presentation, I focus on dissociative chemisorption of N_2 on Ru(0001), examining the impact of vibrational excitations on surface reactivity. Using state-of-the-art gas-surface dynamical modeling with explicit energy exchange [4,5], we computed DC rate coefficients under thermal and plasma conditions. We compared different models that try to quantify the vibrationally enhanced dissociation and analyze their on the micro-kinetic model. Our findings demonstrate that in particular the TST+FM-α model introduces sizable errors for the TOFs [6].

[1] G.-J. Kroes and J. Meyer, Chem. Sci. 16, 480 (2025).
[2] M. Monai *et al.*, ACS Catal. **16**, 4077 (2026).
[3] P. Mehta *et al.*, Nat. Catal. **1**, 269 (2018).
[4] K. Shakouri, J. Behler, J. Meyer, and G.-J. Kroes, J. Phys. Chem. Lett. **8**, 2131 (2017).

[5] P. Spiering, K. Shakouri, J. Behler, G.-J. Kroes and J. Meyer, J. Phys. Chem. Lett. **10**, 2957 (2019).
[6] F. van den Bosch, N. Gerrits, and J. Meyer, EES Catal. **3**, 1257 (2025).

Biography:

Jörg Meyer obtained his PhD at FU Berlin (2012, *summa cum laude*) for modeling energy dissipation during chemical reactions of small molecules on metal surfaces, carried out at the Fritz-Haber-Institute (Max-Planck-Society). During his postdoc time he received two Young Investigator Awards at Gordon Research Conferences. In 2014 he was appointed as an assistant professor in Theoretical Chemistry at Leiden University, where he was granted tenure in 2020. In close collaboration with industrial partners, one of the current research lines in his group is to transfer fundamental insights from gas-surface dynamics regarding elementary reaction steps to applications in heterogeneous catalysis.

Catalysis in Ball Mills: Mechanochemistry as an Alternative Synthesis Strategy

Lars Borchardt*

Ruhr-University Bochum, Germany

Abstract:

We introduce a novel concept of catalysis called direct mechanocatalysis neither utilizing light, thermal heating nor electric potential as in conventional catalysis, but simply mechanical energy. In this mechanochemical approach, mechanical energy is provided by the collision of milling balls inside a ball mill. The catalyst is neither dissolved (as in homogenous catalysis), nor a powder or bed of shaped bodies (as in heterogeneous catalysis), but the milling ball itself. We demonstrate how even in the absence of any solvent, reactants can be brought into reactions mechanocatalytically - only using milling balls that refresh their catalytically active surface constantly during their continuous collisions. We first showcase this concept for a type of reactions that is commonly in the hand of homogeneous catalysis – C-C-cross coupling reactions catalysed by Pd and Cu. We show how various, even sterically-demanding and deactivated reagents, can be converted quantitatively in as little as 60 minutes via Suzuki-, Sonogashira-, Heck-, or Glaser coupling. We further advance this concept to the selective oxidation of alcohols to aldehydes using gold-coated milling balls. Finally we show how even hydrogenation and semi-hydrogenation reactions can be conducted via this approach using milling vessels that are internally coated with Pd, Ru, Ni. By this the hydrogenation of unsaturated C-C and C-O, as well as N-O and C-X bonds is successfully achieved without the use of solvents, ligands, or catalyst powders, but simply via ball milling.

Biography:

Lars Borchardt completed his PhD at TU Dresden and his postdoc at ETH Zurich. He is currently Professor of Inorganic Chemistry at Ruhr University Bochum. His research focuses on sustainable chemistry based on mechanochemistry. In addition to developing new catalytic processes, he investigates the fundamental mechanisms of mechanochemistry.

Sustainable Cross-Coupling Protocol: Miyaura Borylation and One-Pot Suzuki-Miyaura Reaction in Deep Eutectic Solvents (DES)

D. Franchi[1]*, F. D'Amico[1], A. Dessì[1], G. Reginato[1], M. Calamante[1,2], A. Mordini[1,2], L. Zani[1].

[1]National Research Council - Institute of Chemistry of Organometallic Compounds (CNR-ICCOM), Italy; [2]University of Firenze - Department of Chemistry "U. Schiff", Italy.

Abstract:

Within the framework of green chemistry, solvent usage occupies a critical role in designing a new chemical process: Deep Eutectic Solvents (DESs) represent an alternative to common organic solvents.[1] DES are well-suited to green chemistry applications due to their zero-waste synthesis, the use of inexpensive, environmentally benign components, and unique physicochemical properties such as low volatility and high thermal stability. In this work, DESs have been employed as green solvents for Miyaura borylation and Suzuki-Miyaura cross-coupling.[2] To the best of our knowledge, such a one-pot protocol in DES has never been reported in the literature before.[3]

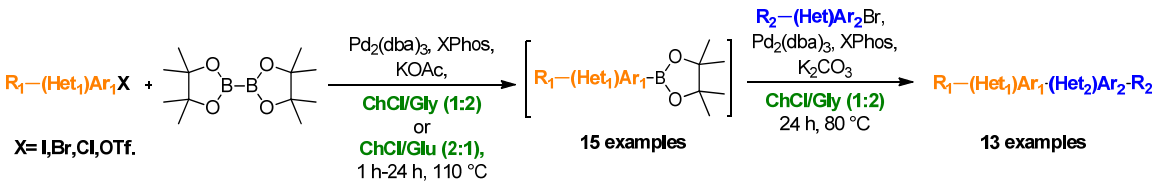

Figure 1. Miyaura borylation and one-pot Suzuki-Miyaura cross-coupling in DES.

Starting from a precedent work on a direct arylation protocol in DES,[4] an optimised protocol for the one-pot Miyaura borylation and Suzuki coupling of (hetero)aromatic iodides, bromides, chlorides, and triflates in choline chloride/glycerol (1:2) and choline chloride/glucose (2:1) DES is presented. The fine-tuning of each reaction component enabled the identification of robust conditions for the borylation of both electron-poor and electron-rich (hetero)aryl substrates with moderate-to-high yields. The obtained boronic esters were isolated and characterised or directly exploited for Suzuki-Miyaura cross-coupling in a one-pot fashion to introduce different bromides. The optimised protocol was successfully applied to easily prepare conjugated organic compounds with potential application in optoelectronics.

The protocol sustainability was established through calculations of green metrics, such as Eco-scale and E-factor, and compared with the literature.

Biography:

[1] A.P. Abbott, G. Capper, D.L. Davies, R.K. Rashed, et al. *Chem. Commun.* **2003**, 70-71.
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[4] F. D'Amico, C. Papucci, D.Franchi, et al. *ACS Sust. Chem. Eng.* **2022**, 10, 9, 3037-3047.

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Use of Zeolites for the Synthesis of Ketals from Ethyl Levulinate and Glycerol

Vincenzo Russo[1,] *, Francesco Taddeo[1], Martino Di Serio[1]

[1]Dipartimento di Scienze Chimiche, Università di Napoli Federico II, Via Cintia, 4, I-80126 Napoli, Italy

Abstract:

The transition toward sustainable chemical processes has stimulated growing interest in biomass-derived feedstocks as alternatives to fossil-based resources. Among these, levulinic acid and its esters are recognized as versatile platform molecules, while glycerol, abundantly produced as a byproduct of biodiesel synthesis, represents an important renewable building block. The acid-catalyzed ketalization of glycerol with ethyl levulinate affords a ketal compound with potential applications as a solvent, plasticizer, and precursor for polymeric materials. A range of solid acid catalysts can promote this transformation, with zeolites being especially attractive due to their high thermal and mechanical stability and robust catalytic properties. In this work, a comparative evaluation of protonated zeolites—HZSM-5, H-Mordenite, H-β, and H-Y—was conducted for the ketalization reaction. The catalysts were systematically characterized with respect to chemical composition, textural parameters, and acid site density. Structure–activity relationships were examined to elucidate the influence of acidity and pore architecture on catalytic performance. All H-form zeolites exhibited high and comparable activity, achieving efficient glycerol conversion, highlighting their suitability as heterogeneous catalysts for biomass-derived ketal synthesis.

Biography:

Prof. Dr Vincenzo Russo, PhD, TkD is an Associate Professor of Industrial Chemistry at the University of Naples Federico II, holding a PhD in Chemical Sciences and a second PhD in Chemical Reaction Engineering. His main research activities deal with kinetic and reactor modeling for biorefinery and water treatment processes. He is an expert in kinetic investigations based on reaction mechanisms and the design of multiphase chemical reactors via multidimensional models. He is the author of 203 international publications with an H-Index of 30.

Value Added Chemicals from Acetylene, Ethylene and Isocyanides by Single to Multi-Cycle Catalytic Processes Using Late Transition Metal Heteroatom Stabilized Singlet Carbene Complexes

Prasenjit Ghosh*

Indian Institute of Technology Bombay, Powai, Mumbai 400076, INDIA

Abstract:

The catalytic conversion of the small-molecule unsaturated substrates like acetylene, ethylene, and isocyanides to value-added targets is an important frontier in the domain of homogeneous catalysis. The talk will highlight our efforts towards this objective using the late transition metal-mediated reactions through iterative mechanistic understandings. Our journey across single-cycle catalyses like the alkyne hydroamination, and hydrohydrazination, to across various multi-component multi-cycle catalyses, namely, three-component amine-aldehyde-acetylene (A3), and azide–isocyanide couplings and the hydrazone-isocyanide-amine (HIA) coupling, will be narrated in keeping with the core theme of our research. Building superior catalysts through enhanced understanding of the catalyst mode of action lies at the heart of our endeavor.

Biography:

Dr. Prasenjit Ghosh is a Professor of Chemistry at IIT Bombay. He received his Ph.D. from Columbia University, New York, in 1998. Following two post-doctoral stints at Brookhaven National Laboratory and the University of California, Santa Barbara, he joined IIT Bombay in 2003. He received the *CRSI Bronze Medal* (2014) from the Chemical Research Society of India and *The Distinguished Lectureship Award* (2011) of the Chemical Society of Japan. He was on the Editorial Advisory Boards of *Organometallics,* (2017-2019), and *Polyhedron,* (2011-2023), and a Subject Editor of *Indian Journal of Chemistry*, (2022-present). His interests lies in organometallics and their applications.

Keynote Talks

Non-Conventional Technologies for Catalyst Preparation and Synthetic Processes

Giancarlo Cravotto

Department of Drug Science and Technology, University of Turin, Via Giuria 9, 10125 Turin, Italy

Abstract:

Non-conventional technologies are increasingly recognised as effective tools for the intensification of catalyst preparation and synthetic processes, offering improved efficiency, reduced energy demand, and enhanced control over material properties. Ultrasound, hydrodynamic cavitation, microwaves, and mechanochemical methods provide alternative activation pathways compared with conventional thermal approaches, enabling faster reactions, improved mass and heat transfer, and, in many cases, lower solvent consumption. In catalyst synthesis, these technologies can promote nucleation, dispersion, particle size reduction, defect generation, and stronger metal support interactions, leading to materials with tailored morphology, higher surface area, and improved catalytic performance. Acoustic and hydrodynamic cavitation dramatically enhance mixing, surface cleaning, and reactive radical formation. Microwave irradiation allows rapid and volumetric heating, improving synthesis reproducibility and reducing processing times. Mechanochemical methods, based on mechanical energy input, enable solvent-free or solvent-minimised synthesis, supporting greener routes for catalyst preparation and chemical transformations. Beyond catalyst design, these technologies can intensify synthetic processes by accelerating reaction kinetics, improving selectivity, and enabling milder operating conditions. Their integration with continuous processing and scalable reactor configurations represents a promising strategy for sustainable chemical manufacturing. This communication will highlight the principles, advantages, and application potential of ultrasound, hydrodynamic cavitation, microwave-assisted processing, and mechanochemistry as complementary approaches for the development of efficient catalysts and intensified synthetic pathways.

Biography:

Prof. Cravotto is Full Professor of Organic Chemistry at the University of Turin since 2005. He has been Director of the Department of Drug Science and Technology since 2007 until October 2018, and vice-Director until October 2024. He is Editor-in-Chief of *Processes* (MDPI). His research activity in the domain of green technologies for process intensification in chemical synthesis, extraction and processing, is documented by more than 630 scientific, peer-reviewed papers (H. Index 90 with over 35,700 citations by Google Scholar) and 25 patents. He collaborates with a variety of industrial partners and he received several national and international awards.

Tuning the Reactivity of Sol-Gel Multifunctional Catalysts for the Synthesis of Added-Value Products

Martino Di Serio[1,*], Serena Esposito[2], Vincenzo Russo[1], Antonio Aronne[3]

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Abstract:

Sol-gel catalysts composition and morphology can be easily tailored to enhance both the reactivity and selectivity towards specific chemical reactions. In the present work it was proven that $Ru_xNb_ySiO_2$ nanomaterials can exhibit excellent performance both in hydrogenation and acid-base catalysis, easily tunable by varying the Ru/Nb ratio. Specific catalytic tests were conducted selecting as model reaction the catalytic hydrogenation of glucose to sorbitol, normally promoted by Ru-based catalysts, and the catalytic conversion of levulinic acid (LA) to γ-valerolactone (GVL), where both the acidity and the reducing power of the catalyst is needed. The hydrogenation and the acid-base activities were demonstrated to be non-linearly dependent on respectively the Ru and Nb content. The different catalytic behaviors were ascribed to the morphological distribution of both Ru and Nb active phases in the gel-derived catalyst. The reduced materials were demonstrated to be effective bifunctional catalysts in the hydrogenation of LA to GVL, as performed under mild conditions and in aqueous environment, and the catalytic performances were not influenced by textural properties of these materials.

In conclusion, the present work represents a fundamental study highlighting how it is possible to easily tune the reactivity of a sol-gel catalyst by adjusting its chemical composition.

Biography:

Prof. Dr Martino Di Serio, PhD, is a Full Professor of Industrial Chemistry at the University of Naples Federico II. His main research activities deal with the synthesis of novel products for biorefinery processes, with special attention to both kinetic and catalytic aspects of the investigated reactions. He is the author of more than 300 international publications with an H-Index of 47.

Invited Talks

Accelerating Green Technologies: The Role of DFT Modeling in Catalyst Design for Low-Carbon Chemical Processes

Izabela Czekaj[1,2]*

[1] *Faculty of Chemical Engineering and Technology, Cracow University of Technology, Warszawska 24, 31-155 Kraków, Poland*

[2] *Interdisciplinary Center for Circular Economy, Cracow University of Technology, Warszawska 24, 31-155 Cracow, Poland*

Abstract:

This talk explores how theoretical modeling is redefining the future of clean chemical technologies. By uniting DFT simulations with next-generation catalyst design, we gain the ability not only to understand reactions but to shape them—creating materials tailored for a low-carbon world. Using green hydrogen production and ammonia cracking as guiding examples, I will discuss how predictive modeling reveals entirely new catalytic pathways, unlocks activity hidden in non-critical materials, and offers a blueprint for zero-emission energy systems. DFT becomes an engine of innovation: compressing years of experimental trial-and-error into months, enabling rational design at the atomic scale, and accelerating the emergence of circular, decentralized energy technologies. The talk will outline a future in which theoretical insights drive transformative solutions, supporting a global transition toward sustainable catalysis and a climate-neutral economy.

Acknowledgments: This work is financially supported by the National Centre for Research and Development (NCBR) under the international CET Partnership program, Research Project No. CETP/2023/60/AMAZE/2025, “AmMoniA as a ZEro-carbon fuel and H2 carrier”. We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centers: ACK Cyfronet AGH, WCSS) for providing computer facilities and support within computational grant no. PLG/2024/017804.

Biography:

Prof. Izabela Czekaj works at the Faculty of Chemical Engineering and Technology at Cracow University of Technology and is a recognized specialist in density functional theory (DFT) and quantum-chemical modeling of heterogeneous catalysts. Her research focuses on mechanistic studies of surface reactions and the computational design of catalysts for ammonia synthesis and cracking, green hydrogen technologies, biomass valorization, and NOx reduction as well as biorefining technologies.

With over two decades of experience, she has advanced the use of theoretical methods in industrially relevant catalysis, supporting the development of low-emission and circular-economy technologies. She has collaborated with leading institutions, including the Paul Scherrer Institute and ETH Zurich, and her work has been published in high-impact journals such as Nature Catalysis and Angewandte Chemie.

Towards the Discovery of Single-Atom Catalysts for Electrochemical Reactions with Atomistic Simulations

Giovanni Di Liberto*

Dipartimento di Scienza dei Materiali, Università degli Studi di Milano Bicocca, Milano, Italy

Abstract:

Single Atom Catalysts (SACs) are emerging as a new frontier in the field, especially for electrocatalytic applications. Computational chemistry offers a valid framework to access the atomistic details of electrocatalytic processes and to rationalize or even predict novel systems. Recently, a lot of attention has been dedicated to the reactions of evolution and conversion of molecular hydrogen and oxygen from or to liquid water.[1] The activity of SACs is usually rationalized or predicted using concepts of heterogeneous catalysis.[2]

In this presentation, we discuss the key ingredients to model catalytic processes on SACs. SACs differ substantially from metal surfaces and can be considered analogues of coordination compounds.[3] We show that this has crucial implications to their properties and reactivity.[4,5] We propose an approach to predict the stability of SACs under working conditions of pH and applied voltage.[6] Needless to say, the adopted DFT functional affects the accuracy of the predictions, and we show evidence suggesting that self-interaction corrected schemes should be adopted.[7] Furthermore, we provide evidence that electrochemical reaction conditions can drive changes to the structure of the active phase with respect to the as-prepared material, explaining the observed reactivity.[8] Last, we discuss ways to detect key reactive species with electrochemical methods and we provide examples on the need to explicitly simulate polarization curves to provide quantitative predictions on the catalytic activity. This work highlights key concepts in single site catalysis[9] and focuses on a few important ingredients to be accounted for when attempting to provide predictions with computational frameworks.

Keywords: *DFT, SACs, HER, OER*

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Quantitative Structure–Reactivity Relationships in Catalytic Biomass Pyrolysis

Tetiana Kulik[1,2*], Borys Palianytsia[2], Alberto Roldan[1], Philip R. Davies[1]

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Abstract:

Establishing quantitative structure–reactivity relationships is a central challenge in the development of efficient catalytic processes for biomass conversion. Catalytic pyrolysis of second-generation biomass and agricultural residues offers a promising route toward the sustainable production of transportation biofuels and value-added platform chemicals.
In this work, nanosized metal oxide catalysts were employed to investigate thermocatalytic transformations of biomass-derived compounds using approaches of physical organic chemistry combined with physicochemical characterization and kinetic analysis. Systematic correlations governing catalytic reactions on oxide surfaces were analyzed within a unified reactivity framework based on Taft and Hammett substituent constants and reaction constants (ρ, ρ*).

Correlations between substituent effects and catalytic reactivity were established using the Linear Free Energy Relationships (LFER) framework supported by experimental kinetic parameters, including the temperature of maximum reaction rate (T_{max}), reaction order (n),

activation energy (E_{act}), pre-exponential factor (v_o), and activation entropy (ΔS_{act}). Semi-empirical models were applied to estimate reaction constants and evaluate kinetic isotope effects.

The proposed approach provides mechanistic insights into key biomass conversion reactions, including catalytic ketonization of fatty acids and the formation of reactive ketenes from model biomass compounds and real waste biomass. These results establish a predictive framework for the mechanistic analysis of catalytic pyrolysis reactions and open new opportunities for the rational design of catalysts for sustainable biomass conversion.

Biography:

Tetiana Kulik is Professor in Chemistry and Physics of Surface. She joined the Cardiff Catalysis Institute in 2023. After studying at Taras Shevchenko National University of Kyiv, she completed a PhD and D.Sc. at the Chuiko Institute of Surface Chemistry, NAS of Ukraine. Her research focuses on catalytic pyrolysis of biomass; applying LFER, TPD-MS, semiempirical methods, and kinetic isotope effects to elucidate surface reaction mechanisms; catalytic upgrading of pyrolysis oil compounds into value-added chemicals and biofuels.

Acknowledgments:

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Ketalization of Ethyl Levulinate with Glycerol Catalyzed by Strata™-XL-C

Francesco Taddeo[1]*, Antonio D'Angelo[1], Rosa Vitiello[1], Rosa Turco[1], Riccardo Tesser[1], Vincenzo Russo[1], Martino Di Serio[1]

[1]*University of Naples Federico II, Department of Chemical Sciences, Italy*

Abstract:

The valorization of biomass for the development of sustainable chemical processes represents a key strategy to replace fossil-based products with renewable alternatives. In this context, levulinic acid and its derivatives play a significant role. The use of esters such as ethyl levulinate allow the avoidance of competitive esterification reactions. Its reaction with glycerol leads to the formation of ketals, versatile compounds with a wide range of industrial applications due to their valuable properties. Catalysis plays a crucial role in this process and can involve either homogeneous catalysts, such as mineral acids, or heterogeneous catalysts. While homogeneous catalysts often provide high conversions, heterogeneous catalysts offer important environmental and operational benefits, including reusability, higher thermal

stability, and easier separation from the reaction medium. This study focuses on the kinetic investigation of the ketalization of ethyl levulinate with glycerol promoted by Strata^{TM}- XL-C as a heterogeneous catalyst. The reaction was investigated both in batch and continuous reactors to evaluate the effect of operating conditions on the reaction rate. The collected data were interpreted through the development of a model which successfully described the experimental results, showing good agreement between the experimental data and the fitted curves.

Biography:

Dr. Francesco Taddeo obtained his PhD in Chemical Sciences in 2022 from the University of Naples Federico II, where he also worked as a research fellow until 2023. Since 2023, he has been an Assistant Professor (RTDa) of Industrial Chemistry at the same university. His research focuses on the valorization of biomass and waste materials for the production of high value-added compounds, with particular emphasis on kinetic studies and heterogeneous catalysis.

Turning Food Waste into Fuel: Sustainable Production of Ethyl Levulinate as Bio-blendstock for Gasoline Engines

Sara Fulignati[1]*, Stefano Frigo[2], Marco Francesconi[2], Luca Miglino[2], Lorenzo Bonaldi[1], Domenico Licursi[1], Claudia Antonetti[1], Anna Maria Raspolli Galletti[1]

[1] Department of Chemistry and Industrial Chemistry, University of Pisa, Italy; [2]Department of Energy, System, Territory and Construction Engineering (DESTEC), University of Pisa, Italy

Abstract:

The transition toward sustainable energy systems requires the synthesis of renewable fuels from waste biomass through sustainable and scalable processes. In this work, bread waste, an abundant by-product of the food supply chain (900 000 ton/year), was valorised through a one-pot acid-catalysed ethanolysis reaction to produce ethyl levulinate (EL), a compound already tested as a bio-additive for Diesel. For the first time, EL synthesis from bread waste was investigated, adopting a cheap catalyst as H_2SO_4 and a high-gravity approach (10 wt% substrate loading), which allows the production of concentrated streams, thus simplifying the separation step and increasing the productivity. The effects of temperature, reaction time, and H_2SO_4 loading were systematically studied to optimize EL yield while minimizing by-products, such as diethyl ether and char. Under the optimized conditions (170 °C, 3 h, 2 wt% H_2SO_4), an EL yield of 57 mol% was achieved together with a char that was characterized by FT-IR and elemental analysis, revealing increased aromaticity and a higher heating value (HHV) of 25.3 MJ/kg, supporting its potential valorisation as a solid biofuel. For the first time, EL was

evaluated as a bio-additive for spark-ignition engines at unprecedented concentrations (20 and 40 vol% in gasoline). Engine tests demonstrated that these blends maintain comparable performance to commercial gasoline, while enabling partial substitution of fossil fuels and leading to the reduction of pollutant emissions. In conclusion, this study demonstrates a circular strategy that integrates food waste valorisation, green catalytic conversion, and sustainable mobility.

Biography:

Dr. Sara Fulignati is a Tenure Track Researcher in Industrial Chemistry at the University of Pisa. Her work focuses on the catalytic valorization of waste biomass and the sustainable production of industrially relevant chemicals, biofuels, and renewable materials according to Green Chemistry principles. She has contributed to numerous peer-reviewed publications and participates in research projects on biomass conversion using innovative catalytic and processing techniques.

DAY-2, JUNE 30, 2026

Keynote Talks

Rational Design of Doped Oxide and Hybrid Nanomaterials for Enhanced Photocatalysis

Stefano Bellucci*

INFN-Laboratori Nazionali di Frascati, Via E. Fermi 54, 00044 Frascati, Italy

Abstract:

The development of efficient and sustainable photocatalysts relies on precise control of material composition, structure, and interfacial properties. This invited talk presents an integrated overview of recent advances in oxide-based and hybrid nanomaterials for photocatalytic applications, with particular emphasis on doped semiconductor thin films and low-dimensional heterostructures.

We first examine the effects of aliovalent doping in CuO and ZnO systems, including Zn-, Al-, and Mg-modified oxides, highlighting how dopant incorporation alters crystallinity, defect density, optical absorption, and charge transport properties, ultimately leading to enhanced photocatalytic degradation of organic pollutants [1–3]. The relationship between

microstructural evolution, band-gap modulation, and photocatalytic efficiency is discussed in detail, supported by complementary experimental and theoretical insights.

The talk then extends to hybrid photocatalysts, focusing on 2D/1D graphene/Ag–Ag_2S nanocomposites, where synergistic effects arising from heterojunction formation, plasmonic contributions, and efficient charge separation result in significantly improved photocatalytic performance [4]. Across these systems, scalable and environmentally benign synthesis strategies are emphasized, together with mechanistic interpretations of light–matter interactions and reactive species generation.

Overall, this contribution outlines a coherent materials-design framework for next-generation photocatalysts, bridging oxide chemistry, nanostructuring, and interfacial engineering for applications in environmental remediation and sustainable catalysis.

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Biography:

Dr. Prof. habil. Stefano Bellucci obtained 1982 Laurea in Physics Degree at Univ. Sapienza Rome (summa cum laude) and 1986 his Ph.D. in Physics of elementary particles at SISSA, Trieste. Research Associate at Brandeis Univ., USA (1983-1985); visiting researcher at M.I.T., Cambridge, USA (1985-1986), at Univ. of Maryland, USA (1986-1987), at Univ. of California at Davis, USA (1987-1988). Tenured Researcher (Research Staff) at INFN (Istituto Nazionale di Fisica Nucleare) Laboratori Nazionali di Frascati (LNF) since 1987. INFN First Researcher (Senior Research Staff) since 2005 (retired in 2024). He published 1000 articles, with 20000 citations, Hirsch index h = 66.

Nanoporous Hybrid Catalysts for Photo(electro)Catalytic Conversion Reactions Across the Carbon, Nitrogen and Water Cycles

Alicia Gomis-Berenguer[1,2] Conchi Ania[2*]

[1] CEMHTI, CNRS (UPR 3079), Université d'Orléans, 45071, Orléans, France

Abstract:

Water, nitrogen, and carbon dioxide are earth-abundant, simple strategic molecules which efficient and sustainable conversion into energy and other added-value chemicals can revolutionize the global energetic scenario, currently dominated by the use of fossil fuels. Solar-driven photocatalytic approaches based on earth-abundant catalysts for the transformation of these molecules seem particularly attractive to boost further advances on the topic. Despite TiO_2 is the benchmark photocatalyst for many applications, its poor activity under natural sunlight has have prompted investigations into alternative semiconductors. Owing to their visible-light absorption ability and low-cost synthesis from sustainable precursors, carbon materials are potential alternatives to transition metal-based semiconductors. Their main cornerstone is the severe recombination of the photogenerated charge carriers. On the other hand, the use of solid-state heterojunctions with semiconductors has proven to be a good strategy to compensate for this limitation. In this communication we report the photocatalytic performance of various carbon material/semiconductor heterojunctions for several reactions of relevance for energy and environmental remediation, covering the carbon, water and nitrogen cycles: i) reduction of CO_2; ii) fixation of N-compounds; iii) water splitting; iv) H_2O_2 generation. ***Acknowledgements***: European Research Council (ERC-CoG 648161), region Centre Val de Loire (MATHYFON) and ANR (ZENITH) programs.

Biography:

Dr. Conchi ANIA (PhD 2003) is a Research Director of CNRS (France) and Research Scientist of CSIC (Spain). She has a long-standing interest on nanoporous carbons with tailored surface chemistry and architectures for applications in energy conversion and storage and environmental remediation (adsorption, photocatalysis, electrocatalysis). She has coauthored over 170 scientific publications with over 9000 citations (H_{index} 53). In 2008 she received the national L'Oreal-Unesco Research Fellowship "For women in Science". In 2023 she received the Silver Medal of CNRS. She is Editor of Carbon journal (Elsevier) since 2020.

Invited Talks

Hydrogen Production from Aqueous Organic Solutions *via* Solar Thermo-Photoreforming over Semiconductor/Carbon Photocatalysts

Giuseppe Marcì[1*], Khalil Abbassi[1], Elisa I. García-López[1], Conchi Ania[2]

1 Department of Engineering (DI), University of Palermo, Palermo, Italy
2 POR2E Group, CEMHTI CNRS (UPR 3079), Université d'Orléans, 45071 Orléans, France]

Abstract:

Solar energy conversion into H_2 offers a promising route to address global sustainability challenges. Photoreforming enables hydrogen production from aqueous biomass-derived organics by using illuminated photocatalysts that reduce protons to H_2 while oxidizing organic substrates. Nb_2O_5 exhibits activity comparable to commercial TiO_2 in this reaction. To enhance its performance, hybrid semiconductor/carbon catalysts have been developed, where the semiconductor drives photocatalysis and the carbon acts both as an electron reservoir, improving charge transfer, and as an infrared absorber to better exploit the solar spectrum. Home prepared Nb_2O_5 and commercial TiO_2 (P25), along with composites containing 5 to20 wt% carbon, were prepared, characterized, and tested for photo(thermo)reforming of aqueous glycerol. Carbon phases included graphene, graphene oxide and carbon xerogels.

Biography:

Giuseppe Marcì is Full Professor of Chemistry at the Department of Engineering, University of Palermo (UNIPA). His research focuses on the development of advanced materials for sustainable energy and environmental applications, including heterogeneous catalysis and photocatalysis for green and sustainable processes, biomass valorization, and advanced oxidation technologies. He is author of more than 160 papers H-index 54, editor of an Elsevier book “Heterogeneous Photocatalysis: Relationships with Heterogeneous Catalysis and Perspectives” 2019 and co-author of chemistry didactical texts as “Elementi di Chimica” and “Stechiometria” edited by Edises.

Photocatalytic Energy Conversion with Nanostructured Semiconductors

Kei Noda*

Keio University, Department of Electronics and Electrical Engineering, Yokohama, Japan

Abstract:

Photocatalytic energy conversion such as water splitting and carbon dioxide (CO_2) reduction have been widely researched to contribute to both the production of renewable energy sources and the reduction of greenhouse effect gases, where materials development of supreme photocatalysts has been strongly demanded. In the past several years, our group has performed continuous research on nanostructured photocatalysts such as vertically aligned titanium dioxide (TiO_2) nanotube arrays, cuprous oxide (Cu_2O) nanoparticles, and tungsten trioxide (WO_3) nanorods [1-3]. In addition, polymeric carbon nitrides, represented by g-C_3N_4 and C_3N_5 that can be classified as n-type polymer semiconductors, are promising as one of visible-light-responsive photocatalysts because of its high thermal and chemical stability, and metal-free chemical composition [2-4]. In this presentation, our recent results on

photocatalytic hydrogen and fuel production by CO_2 reduction using Z-scheme (or S-scheme) based composite photocatalysts made of nanostructured semiconductors will be introduced. Besides, I will also mention the uniform deposition of g-C_3N_4 nanoparticles on TiO_2 nanotube arrays with the aid of our originally developed thermal chemical vapor deposition system, which is quite effective for improving the performance of nanostructured composite photocatalysts [3].

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Biography:

Kei Noda received the doctoral degree from Kyoto University, Japan, in 2002. After working as a Humboldt foundation research fellow at the Max Planck Institute for Solid State Research and as an assistant professor at the Graduate School of Kyoto University, he became a lecturer and an associate professor in the Department of Electronics and Electrical Engineering at Keio University, Japan, in 2013 and 2015, respectively. He has been a full professor in the same department since April 2021. His research interests include physical properties and application of various semiconductors such as carbon-based materials and metal oxides.

TaNbHfZrTi High-Entropy Alloy in Photo(electro) Catalytic Tetracycline Degradation

Lara Einfalt[1,2], Bor Arah[3], Sandra Drev[3], Barbara Podmiljšak[1,2], Petr Hruška[4,5], Stefan Andrei Irimiciuc[4], Stanislav Cichoň[4], Dejan Prokop[4,5], Ján Lančok[4], Belisa Alcantara Marinho[3], Miran Čeh[1,3*]

[1]Jožef Stefan Institute, Department for Nanostructured Materials, Slovenia, [2]Jožef Stefan International Postgraduate School, Slovenia, [3]Jožef Stefan Institute, Center for Electron Microscopy and Microanalysis, Slovenia, [4]Institute of Physics of the Czech Academy of Sciences, Czechia, [5]Charles University, Faculty of Mathematics and Physics, Czechia

Abstract:

High-entropy materials (HEMs) have recently gained attention in catalysis due to their unique structural and electronic properties. Composed of five or more elements in a single-phase lattice, these materials exhibit lattice distortions, uneven electron distribution, and oxygen vacancies, which can enhance catalytic performance. In this study, anodically treated TaNbHfZrTi high-entropy alloys (bulk, thin films) were used for photocatalytic (PC), electrocatalytic (EC), and photoelectrocatalytic (PEC) degradation of tetracycline. Both, bulk

TaNbHfZrTi alloy and magnetron-sputtered TaNbHfZrTi thin films were anodized at various voltages for different times and subsequently annealed at temperatures up to 1000°C. Microstructural analysis using various advanced SEM and TEM techniques (FIB-prepared lamellas, TEM heating experiments) was used to study the chemical composition of anodized structures, as well as their degree of crystallinity and morphology. SEM and TEM of anodically treated TaNbHfZrTi showed that the anodic oxidation process of bulk and thin film TaNbHfZrTi caused amorphization of the surface in the form of ordered nanotubular structures in bulk TaNbHfZrTi or sponge-like structures in thin film TaNbHfZrTi. After thermal treatment, both morphological features were transformed into crystalline oxides, suggesting that anodization and subsequent thermal treatment can directly transform metal TaNbHfZrTi into oxide. Degradation tests of tetracycline showed that amorphous samples achieved up to 60% PC degradation within one hour. Furthermore, EC and PEC performance improved with increasing applied voltage and film reuse, with PEC reaching up to 80% degradation after three hours. These findings highlight the strong potential of TaNbHfZrTi and related HEMs as effective photo(electro)catalysts for antibiotic pollutant removal.

Biography:

Miran Čeh has extensive expertise in the investigation of the structure and chemical composition of materials using advanced electron microscopy techniques at the micro-, nano-, and atomic levels. More recently, he has been involved in studies of new generation materials for catalytic applications. He is a scientific advisor at the Nanostructured Materials Dpt. at the JSI, a full professor at the Faculty of Chemistry and Chemical Engineering at the University of Maribor, and at the Jožef Stefan International Postgraduate School. He is also the head of the Center for Electron Microscopy and Microanalysis (CEMM) at the JSI.

Nitrate Radicals in Photocatalysis: An Emerging Tool for Selective Oxidation [Online]

Alessandro Gottuso[1,2]* and Francesco Parrino[2]

[1]School of Environmental Science and Engineering, Shanghai Jiao Tong University, China
[2]Department of Industrial Engineering, University of Trento, Italy

Abstract:

Although nitrate radicals (NO_3) are well known in atmospheric chemistry, their role in photocatalysis remains comparatively underexplored as selective oxidizing intermediates. In contrast to less selective radical pathways, nitrate radicals can enable controlled oxidation chemistry under mild conditions, making them attractive for both organic synthesis and environmental remediation. Recent advances in catalytic materials and reaction engineering have made it possible to promote NO_3 generation from nitrate-containing systems under light

irradiation and to investigate its reactivity through dedicated mechanistic and radical-detection approaches. Such reactivity is particularly relevant to selective olefin oxidation, where nitrate-radical-mediated pathways open access to valuable products. At the same time, the same reactive platform can be directed toward degradation of recalcitrant pollutants, highlighting the broader scope of this chemistry beyond synthesis. On top of that, the extension from purely photocatalytic operation to electro-assisted configurations further expands these opportunities, as the application of an external bias offers improved control over charge separation, interfacial redox steps, and reaction selectivity, while avoiding sacrificial additives. Overall, nitrate-radical chemistry is emerging in photocatalysis as a versatile strategy for developing selective and sustainable processes.

Biography:

Alessandro Gottuso is a postdoctoral researcher at Shanghai Jiao Tong University, where he works on the development of COF materials for decentralized H_2O_2 photosynthesis. He received his PhD, with Doctor Europaeus distinction, from the University of Trento in 2025. His research interests also include the development of novel photo(electro)catalytic procedures for selective redox processes, biomass valorization, and environmental remediation, combining materials design and mechanistic investigation with spectroscopic and electrochemical techniques to elucidate charge-transfer processes and identify reactive intermediates.

Recent Advances in Single Nanowire Photodetector

Priyanka Ramaswamy*

Micron Technology, USA

Abstract:

In this talk, the recent development in single nanowire next-generation photodetectors will be discussed. Primary focus of the talk will be on structural engineering, conduction mechanisms of the different types of detectors and core challenges of the nanostructure. Finally, single nanowire-based applications in various fields such as electronic devices, photonics for quantum technology, and robotics will be summarized.

Biography:

Dr. Priyanka Ramaswamy is a Staff Process Integration Engineer at Micron Technology, USA. She earned her Ph.D. in Electrical Engineering from North Carolina A&T State University, USA, where her research focused on advanced electronic materials and semiconductor

technologies. Her academic and industrial experience spans semiconductor device engineering, process integration, and materials characterization.

Dr. Ramaswamy's research interests include semiconductor manufacturing, electronic materials, and device optimization for next-generation technologies. She has authored more than ten peer-reviewed research publications and is the inventor of a pending U.S. patent. Through her work in both academia and industry, she contributes to the advancement of innovative semiconductor processes and high-performance electronic devices.

Eco-Friendly and Reusable CNT/Halloysite-Based Sensor for Ciprofloxacin Electrochemical Detection

Carlo Spampinato*[1], Ivana Caruso[1,2], Viviana Scuderi[1], Simona Filice[1], Silvia Scalese[1]

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[2]Università degli Studi di Catania, Dipartimento di Fisica ed Astronomia, Via Santa Sofia, n.64, Catania, 95125, Italy

Abstract:

The development of sustainable interfaces able to couple selective molecular capture, efficient charge transport, and light-assisted surface renewal is highly attractive for environmental monitoring. Here we report a CNT/halloysite-based hybrid platform that operates as an electrocatalytically active and regenerable interface for ciprofloxacin detection in water. Commercial carbon screen-printed electrodes were modified by multilayer drop-casting of fully aqueous dispersions of multiwalled carbon nanotubes and halloysite nanotubes, yielding a simple, scalable, and solvent-minimized fabrication route. This hybrid architecture exploits the high conductivity of CNTs and the adsorption ability of halloysite, improving charge transfer and increasing ciprofloxacin concentration at the electrode surface. Among the investigated configurations, the CNT-HTA-X5 electrode delivered the best performance, showing the lowest charge-transfer resistance, the highest oxidation response toward ciprofloxacin, a linear response in the 4.25–34 µM range, and a limit of detection of 61 nM. Beyond sensitivity, the most distinctive feature of the platform is its photo-assisted regeneration: after fouling by adsorbed antibiotic, the original electrochemical response is restored by short UVA irradiation, enabling repeated sensing cycles on the same device. This behavior points to a synergistic interplay between adsorption-driven interfacial enrichment and light-triggered surface cleaning, opening a promising route toward reusable catalytic sensing materials. The proposed CNT/halloysite interface therefore offers an attractive balance of analytical performance, low-cost processing, and green design for next-generation monitoring of emerging pharmaceutical contaminants.

Biography:

Carlo Spampinato is a Researcher at CNR-IMM, Catania, working at the interface of nanomaterials, electrochemistry, and sustainable energy technologies. He received his PhD in Physics in 2025, focusing on perovskite solar cells, transparent oxide thin films, and green functional materials. His current research includes nanostructured electrodes, electrochemical impedance spectroscopy, and voltammetric sensing. His scientific activity aligns with the conference themes of catalysis, advanced materials, and environmental sustainability, with applications spanning renewable energy, pollutant monitoring, and green analytical technologies.

An Operando Study of the Surface Chemistry of (Ni,Cu)-Catalysts for Bio-Ethanol Dehydrogenation Reaction

Elena Spennati1,2,*, Giovanni Pampararo3, Gabriella Garbarino1,2, Paola Riani2,3

1University of Genova, DICCA Dept., Genova, Italy
2 INSTM, UDR Genova, Genova, Italy
3 University of Genova, DCCI Dept., Genova, Italy

Abstract:

In the energy transition scenario, it is crucial to develop environmentally friendly processes instead of fossil-based ones. One interesting process is bio-ethanol dehydrogenation to produce bio-acetaldehyde, which has the advantage of producing one of the main petrochemical products used as a flavoring agent in food engineering. The main challenge of this process is developing a robust, selective, and stable catalyst. In this contest, this study investigates the bioethanol dehydrogenation process using a (Cu,Ni) catalyst supported on Al2O3, considering the effects of the preparation procedure (solid combustion synthesis or hydrothermal impregnation) and thermal treatment. Furthermore, an operando DRIFTS study was performed to evaluate molecular-scale phenomena, to determine intermediate species and reaction mechanisms, with the aim of gaining an understanding of possible catalyst deactivation. (Cu,Ni)-based catalysts were found to be more active than Cu-based ones, particularly at temperatures lower than 573 K, in terms of both ethanol conversion and acetaldehyde selectivity. Pre-reduction treatment significantly improved the catalytic performance of the dehydrogenation reaction without altering the high-temperature activity, where the alumina's classical activity prevails. A catalyst surface study under operando conditions revealed that ethoxide and acetate species predominate on both the Al3+ of the support and the metallic Cu. Ni introduction decreased the intensity of bands related to the acetate species on Cu, suggesting a lower interaction. Furthermore, according to obtained

data, the acetate groups act as spectators in the dehydrogenation reaction and are one of the main causes of catalyst deactivation.

Biography:

Elena Spennati is a tenure track researcher in industrial technological chemistry (ICHI-02/B) at the Department of Civil, Chemical, and Environmental Engineering, University of Genoa. She has an h-index of 12 and has published 28 documents with over 400 citations. Her main research interests include the development and optimization of innovative heterogeneous catalysts and catalytic processes for green chemistry, particularly for CO2 utilization reactions and renewable hydrogen production.

Oriented WO3 Nanoflakes Immobilized on Glass Spheres for the Continuous Flow Photocatalytic Degradation of Pharmaceuticals

Vito Cristino[1]*, Claudia Stevanin[1], Tatiana Chenet[1], Luisa Pasti[1], Stefano Caramori[2]

[1]Department of Environmental and Prevention Sciences, University of Ferrara,Italy;

[2]Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara, Italy

Abstract:

In recent years, the quality of aquatic environments has been increasingly compromised by emerging contaminants (ECs), particularly pharmaceuticals such as antibiotics and anti-inflammatories. Conventional wastewater treatment plants (WWTPs) often fail to efficiently remove these compounds, leading to environmental toxicity and the spread of antibiotic resistance. This study presents an innovative strategy for water remediation using advanced oxidation processes (AOPs) in a continuous flow system. We developed a photocatalytic system based on solvothermally grown WO_3 nanoflakes immobilized on the inert surface of glass spheres.

Structural and photoelectrochemical characterization confirmed that these oriented lamellar arrays provide superior stability, photocurrent generation, and charge separation compared to standard WO_3 nanoparticles. Unlike many other semiconductors, WO_3 produces hydroxyl radicals (•OH) capable of oxidizing most of organic molecules; thus, the oxidation of organic compounds can proceed via two primary pathways: direct oxidation by photogenerated holes or mediated by hydroxyl radicals. The photocatalytic efficiency was compared using suspension-based batch experiments and immobilized catalyst continuous flow configurations for the degradation of different target pharmaceuticals. The reaction was monitored to assess the complete mineralization of organic pollutants. LC/MS analysis was performed to monitor degradation kinetics and identify transformation products, demonstrating the efficacy of the

laboratory-scale plant. While batch experiments showed faster kinetics, the continuous flow reactor prototype offers a robust and scalable solution for treating large volumes of contaminated water, overcoming the recovery limitations associated with suspension-based catalysts.

Biography:

Vito Cristino is a Tenure Track Researcher in General and Inorganic Chemistry at the University of Ferrara, Italy. His work focuses on the scalable synthesis and characterization of nanostructured materials on various substrates, specifically targeting semiconductors for the Oxygen Evolution Reaction (OER) and the functionalization of these photoactive interfaces with water oxidation catalysts (WOCs). These systems are developed for applications in solar energy conversion, water splitting, and environmental remediation. He has contributed to several national and international research projects, and his scientific activity includes numerous peer-reviewed publications and international patents.

Nanocatalysts for Lignocellulosic Biomass Conversion toward Pharmaceutical Building Blocks

Alina M. Balu[1]*, Olena Korchuganova[1], and Alexander Pokutsa[1]

[1]*University of Córdoba, Spain, Organic Chemistry Department*

Abstract:

In the SusPharma project, one of the most impactful research lines for advancing pharmaceutical development is the design of new catalysts and their integration into continuous-flow reactors. Catalyst development focuses on optimizing processes that use lignocellulosic biomass as a renewable raw material for producing pharmaceutical intermediates. This biomass is composed of hemicellulose, cellulose, and lignin, all of which can be transformed into valuable building blocks essential for drug synthesis.

A complete process has been established for the separation of hemicellulose and its conversion into monosaccharide solutions, many of which are suitable for downstream chemical transformations. Among these sugars, xylose is of particular interest because it serves as a precursor to furfural, a key platform molecule widely used as a starting point for the synthesis of various pharmaceuticals.

Several catalytic synthesis protocols have been developed, including metal oxides, metal oxalates, and biochar-derived materials. An efficient catalyst for converting D-xylose into furfural has been obtained, enabling a faster and more environmentally friendly process. In addition, the reductive amination of biomass-derived substrates has been achieved using the

Ru-HC catalyst to produce nitrogen-containing molecules. Acid-functionalized nitride materials—such as sulfonated graphitic carbon nitride (SGCN) and sulfonated boron nitride (SBN)—have been successfully synthesized and applied in the conversion of furfuryl alcohol into alkyl levulinates.

The project team is currently working on incorporating these catalysts into flow reactors in the form of 3D-printed structures, in collaboration with the consortium partner VITO. Furthermore, newly developed nanoscale catalysts have been tested for photocatalytic reactions using the Photocube reactor.

Biography:

Alina M. Balu earned her PhD in Fine Chemistry from the University of Córdoba, Spain, in 2012 where she now serves as Associate Professor. Her work focuses on the design of nanomaterials for catalytic applications in producing fine chemicals and biofuels. She has pioneered methods such as microwave-assisted deposition, co-precipitation and mechanochemical synthesis. Dr Balu has held a Marie Curie Fellowship at Avantium (Netherlands), worked at Aalto University (Finland), and received the Green Talent Award from Germany's BMBF. As a member of the NANOVAL group, she currently leads the University of Córdoba's contribution to Horizon Europe projects Suspharma and GreenDigiPharma.

Oral Talks

Bio-Based LICL-Containing Hydrogel Electrolytes for Sustainable Energy Storage: Structure-Efficiency Relationships

Quentin De Roover1*, Aurore Richel1

1 Laboratory of Biomass and Green Technologies, Gembloux Agro-Bio Tech, University of Liege, B-5030 Gembloux, Belgium

Abstract:

The development of safer and more sustainable electrolytes is a key challenge for next-generation of energy storage. In this work, we investigate bio-based hydrogels composed of starch, poly(vinyl alcohol) (PVA), and gluten, incorporating lithium chloride (LiCl) as an ionic charge carrier. These materials are designed as environmentally friendly alternatives to conventional carbonate-based liquid electrolytes. The relationship between the physicochemical structure of the hydrogels and their ionic conductivity is explored using a multi-technique approach. Ionic conductivity are evaluated by electrochemical impedance

spectroscopy (EIS), while differential scanning calorimetry (DSC) provides insights into thermal transitions. Rheological measurements (amplitude and frequency sweeps) are used to assess the viscoelastic network structure, which plays a critical role in ion mobility. Complementary structural analyses are performed using ATR-FTIR spectroscopy to probe molecular interactions between polymer chains and lithium ions, and X-ray diffraction to evaluate the degree of crystallinity and its influence on ion transport pathways. The results obtained contribute to a better understanding of bio-based hydrogel systems containing lithium salts and provide a basis for discussing how their structural and physicochemical characteristics may relate to ion transport properties. This study highlights the potential of bio-based hydrogels as promising solid-like electrolytes for sustainable energy storage applications and provides fundamental insights into the design of next-generation green electrolytic systems.

Biography:

Quentin De Roover is a PhD student at the University of Liège in Agricultural Sciences and Biological Engineering. He obtained a Master's degree in Chemical Sciences from the University of Mons. His research interests include bio-based materials and hydrogel systems for electrochemical applications.

Enhancing Photocatalytic Hydrogen Production: Modification of TiO_ by Coupling with Semiconductor Nanoparticles

Saud Alshammari*

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Abstract:

Photocatalytic water splitting to produce hydrogen (H_2) has obtained significant attention as an environmentally friendly technology. This process, which produces hydrogen from water and sunlight, represents a renewable energy source. Titanium dioxide (TiO_2) plays a critical role in photocatalytic hydrogen production due to its chemical stability, availability, and low cost. Nevertheless, TiO_2's wide band gap (3.2 eV) limits its visible light absorption and might affect the effectiveness of the photocatalytic. Coupling TiO_2 with other semiconductors is a strategy that can enhance TiO_2 by narrowing its band gap and improving visible light absorption. This paper studies the modification of TiO_2 by coupling it with another semiconductor such as CdS nanoparticles using a reflux reactor and autoclave reactor that helps to form a core-shell structure. Characterization techniques, including TEM and UV-Vis spectroscopy, confirmed successful coating of TiO_2 on CdS core, reduction of the band gap from 3.28 eV to 3.1 eV, and enhanced light absorption in the visible region. These modifications are attributed to the heterojunction structure between TiO_2 and CdS.The

essential goal of this study is to improve TiO_2 for use in photocatalytic water splitting to enhance hydrogen production. The core-shell TiO_2@CdS nanoparticles exhibited promising results, due to band gap narrowing and improved light absorption. Future work will involve adding Pt as a co-catalyst, which is known to increase surface reaction activity by enhancing proton adsorption. Evaluation of the TiO_2@CdS@Pt catalyst will include performance assessments and hydrogen productivity tests, considering factors such as effective shapes and material ratios. Moreover, the study could be enhanced by studying further modifications to the catalyst and displaying additional performance evaluations. For instance, doping TiO_2 with metals such as nickel (Ni), iron (Fe), and cobalt (Co) and non-metals such as nitrogen (N), carbon (C), and sulfur (S) could positively influence the catalyst by reducing the band gap, enhancing the separation of photogenerated electron-hole pairs, and increasing the surface area, respectively. Additionally, to further improve catalytic performance, examining different catalyst morphologies, such as nanorods, nanowires, and nanosheets, in hydrogen production could be highly beneficial. Optimizing photoreactor design for efficient photon delivery and illumination will further enhance the photocatalytic process. These strategies collectively aim to overcome current challenges and improve the efficiency of hydrogen production via photocatalysis.

Catalytic Decarboxylation of Lignin-Derived Cinnamic Acids

Tetiana Kulik[1,2], Borys Palianytsia[2*], Nataliia Nastasiienko[2], Max Quayle[1], Mykola Ilchenko[2,3], Greg Shaw[1], Alberto Roldan[1], Duncan Wass[1], Philip R. Davies[1]

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Abstract:

Recent advances in lignin depolymerization technologies have enabled the production of bio-derived *p*-hydroxycinnamic acids in significant quantities, opening new opportunities for sustainable valorization of lignocellulosic biomass. Understanding the mechanisms of their catalytic decarboxylation to valuable 4-vinylphenols is critical for developing green and efficient upgrading strategies.

In this work, catalytic pyrolysis of bioderived cinnamic acids was investigated as model reactions of lignin H-, G-, and S-units on nanosized metal oxide catalysts (nanoceria, alumina). Reaction mechanisms were studied using TPD-MS, IR and UV–Vis spectroscopy, XPS, DTG/TGA/TG, complemented by atomistic simulations.

Kinetic parameters of the decarboxylation reaction on nanosized oxide surfaces were determined. Analysis of IR spectra, including *in situ* measurements, revealed the formation of surface complexes responsible for decarboxylation, mainly monodentate and bidentate chelating carboxylates on both alumina and nanoceria surfaces. Based on experimental kinetic data and theoretical calculations, plausible mechanisms of catalytic decarboxylation were proposed.

DFT calculations indicate that acid-catalyzed decarboxylation of bioderived *p*-coumaric, ferulic, and sinapic acids is the most energetically favorable pathway leading to valuable 4-vinylphenols, including 4-vinylphenol, 4-vinylguaiacol, and canolol. Atomistic modeling further shows that parallel adsorption of sinapic acid on nanoceria is preferred, while transition-state modeling suggests an intramolecular decarboxylation pathway consistent with experimental activation energies.

These findings underscore the key role of catalyst surface chemistry in steering selective, sustainable biomass pyrolysis toward aromatic platform chemicals.

Biography:

Borys Palianytsia is a Researcher in the Laboratory of Kinetics and Mechanisms of Chemical Transformations on Solid Surfaces at the Chuiko Institute of Surface Chemistry, NAS of Ukraine. He is an expert in mass spectrometry, temperature-programmed desorption mass spectrometry (TPD-MS), vacuum systems, and high-temperature experimental techniques. His research focuses on advancing TPD-MS instrumentation and methodologies for studying pyrolysis kinetics and elucidating mechanisms of catalytic pyrolysis reactions.

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Invited Talks

Sequential Catalytic Incorporation of CO_ and CO Leading to Carbonylated Cyclic Carbamates

Lucia Veltri*, Ifeoma Juliet Ozoemena and Bartolo Gabriele

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Abstract:

The catalytic incorporation of both CO and CO_2 into an organic substrate able to cyclize is a very attractive approach to the synthesis of functionalized heterocycles, however, it is a difficult task to accomplish owing to the need for simultaneous activation of both carbon oxides.[1-3]

We report here two innovative examples of catalytic incorporation of CO_2 and CO into acetylenic amines (2-ethynylanilines **1** and propargylic amines **3**) that have enabled the direct and multicomponent synthesis of heterocyclic derivatives of particular interest (functionalized 1,4-dihydro-2*H*-benzo[*d*][1,3]oxazin-2-ones **2** and oxazol-2(3*H*)-ones **4**, Schemes 1 and 2, respectively). Reactions have been performed in the presence of the simple PdI_2/KI catalytic system[4] under oxidative aminocarbonylation conditions[5] (cocatalysis of Ag(I) and DBU was also needed in the case of 2-ethynylanilines, Scheme 1). The new synthetic processes proceed through PdI_2-catalyzed oxidative carbamoylation of the triple bond of substrates followed by in situ carboxylative cyclization.

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Catalytic Conversion of CO_ and CH_ into Acetic Acid and Formic Acid Through Ni__ Clusters Supported on MgO Surface: A DFT Study

Aravindhan Ramachandran* and Sergio Tosoni

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Abstract:

Catalytic conversion of CO2 and CH4 to obtain essential chemicals is a promising way of utilizing carbon resources to diminish CO2 emissions and to mitigate global warming. For the catalytic conversion, metal catalyst plays a commendable role in the catalytic activity with the good activation capabilities. In this regard, nickel clusters gain huge attention with prominent catalytic activity and higher natural abundance. Our computational investigation performed

through density functional theory calculations provides the possible reaction pathways to obtain acetic acid and formic acid by catalytic conversion of CO2 and CH4 gases through Ni13 clusters and MgO surfaces. Our results evidence the strong adsorption of CO2, CH4 and their intermediates on the Ni13 clusters deposited on the MgO surface. Our work also witnessed the oxidized Ni13 clusters are more stable and prominent for the catalytic activity. On MgO thin films supported on Ag, thermodynamically favorable reverse oxygen spill over facilitates the oxidation of Ni13 clusters through excess oxygens trapped between the Ag(100) and MgO surfaces. Catalytic conversion reactions carried out on the oxidized Ni13 clusters placed on the MgO and Ag(100) surface also exhibit prominent adsorption and validates the reactions pathways in both unoxidized and oxidized Ni13 clusters.

Biography:

Aravindhan Ramachandran is a postdoctoral researcher in Computational Surface Science Lab headed by Prof. Sergio Tosoni, Department of Material Science, University of Milano Bicocca, Milan. His research focusses on the catalytic activity of metal clusters and Cluster-Surface interactions. He finished is Ph.D. in computational chemistry from Vellore Institute of Technology, Vellore, India.

Zn-based Electrocatalysts for CO_2 Utilization: From Controlled Synthesis to Mechanistic Understanding and Efficient Devices

Nataly Carolina Rosero-Navarro*, Elías Rodríguez-Jara and Mario Aparicio

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Abstract:

The development of efficient and scalable electrocatalysts for the CO_2 reduction reaction (CO_2RR) requires not only high catalytic performance but also a deeper understanding of the structure–activity relationships governing reaction pathways under realistic operating conditions. This work presents a comprehensive study of ZnO-based electrocatalysts synthesized through different routes and surface modifications to establish direct correlations between synthesis strategy, surface properties, and CO_2RR performance. ZnO provides a versatile platform for tailoring surface chemistry, crystallographic orientation, and catalytic behaviour through controlled synthesis. Among the investigated materials, microwave-assisted solvothermal synthesis produced ZnO nanorods with the most promising performance, combining rapid and sustainable synthesis with remarkable selectivity toward CO production. This approach enabled the formation of highly crystalline and homogeneous nanostructures with controlled anisotropic growth and enhanced exposure of catalytically relevant crystal planes, resulting in significantly improved CO_2 conversion compared to

conventionally synthesized counterparts. The catalysts were successfully integrated into gas diffusion electrodes and evaluated in both conventional electrochemical systems and zero-gap cell architectures, demonstrating their potential for scalable CO_2-to-CO technologies. Additionally, operando-inspired spectro-electrochemical methodologies were implemented to investigate active sites and reaction intermediates during CO_2RR.

Biography:

Nataly Carolina Rosero-Navarro is a Tenured Scientist at the Institute of Ceramics and Glass since 2022 and Guest Associate Professor at Hokkaido University. She obtained her Ph.D. in Chemical Sciences from the Autonomous University of Madrid in 2011 and completed postdoctoral research with a Japan Society for the Promotion of Science fellowship. Her research focuses on inorganic and hybrid materials for environmental and energy applications, particularly green energy generation and storage. She received the WinGS Women in Global Science Award (2017) and the Ulrich Award (2022).

NAP-XPS Study of CO and CO_ Hydrogenation on Ni(111) Under h-BN Cover [Online]

Giovanni Carraro [2] , Masaaki Ando [3], Marco Smerieri [2], Michio Okada [3], Gabriella Garbarino [4], Letizia Savio [2] , Mario Rocca [1,2] , Luca Vattuone [1,2] *

[1] DIFI University of Genoa, Italy, [2] IMEM CNR, Italy, [3] Dep. Of Chemistry, University of Osaka Japan, [4] DICCA University of Genoa, Italy.

Abstract:

The methanation of CO and CO_2 in excess H_2 over Ni is an important reaction occurring readily at high pressures for which no complete understanding of the active mechanisms has been achieved so far. X-Ray photoemission spectroscopy (XPS) in *operando* conditions might, in principle, unravel the different reaction steps, but unfortunately complete hydrogenation of C could not achieved even close to ambient pressure (AP) conditions. Following the indication that this process is favored in presence of a h-BN cover on Ni nanoparticles, we explored the methanation reaction under Near Ambient Pressure (NAP) conditions up to 10 mbar on h-BN covered Ni(111).

Our results show the hydrogenation steps leading to CH_x formation at 30 times lower pressure than in absence of the h-BN cover, confirming the effectiveness of the confinement of the reactants. CO and CO_2 share a common path leading to HCO and its dissociation and the hydrogenation of its fragments are the rate limiting steps. The oxygen atoms released in the reaction react thereby with the h-BN cover leading to the formation of boron oxides. Above

230 °C the Reverse Water Gas Shift reaction is observed, which is indeed favored with respect to methanation in agreement with previous studies.

Biography:

L.V. got his PhD in Physics at the University of Genoa in 1994. After a post-doc at the University of Cambridge (UK) with Sir D.A. King he returned to Genoa. Since 1999 he is a staff Researcher at Unige, and since 2012 Associate Professor.
L.V. research covers experimental studies of gas-surface interaction using vibrational spectroscopy, single crystal calorimetry, supersonic molecular beams and XPS.
Recently his activity focused on the chemical reactivity of graphene and 2D materials and on confined chemistry. L.V. is now Section editor of Coatings and Associate Editor of Frontiers in Chemistry.

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Anthocyanins as Natural Sensitizers of TiO_2 Thin Films: Optical and Electrochemical Characterization

William Vallejo[1]*, Carlos Diaz[1], Maria Villareal[1]

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Abstract:

Titanium Dioxide (TiO_2) is one of most studied semiconductors in the field of photocatalysis. Due to its wide band gap value, the TiO_2 is only photo-active under UV irradiation. Different strategies have been developed to extend its photocatalytic properties into the visible region of the electromagnetic spectrum.[1] Among different modification strategies, the sensitization has demonstrated potential for improving the photocatalytic performance of TiO_2. The sensitization can be achieved using synthetic or natural dyes. In general, synthetic dyes reported best performance; however, they are expensive and harmful to the environmental. In contrast, natural dyes are a more sustainable alternative, as they are cheap and biodegradable.[2] The performance of catalytic system based on natural dyes as sensitizers is lower than reported to the synthetic dyes. However, natural sensitizers are an environmentally sustainable alternative as they can contribute in the medium term to the development of sustainable solutions for water cleaning and energy production.[3] In this work, we fabricated TiO_2 thin films using anthocyanins obtained from local specie called “corozo”. The thin films were fabricated by using Doctor Blade technique, and chemisorption was employed as sensitization method. The samples were characterized by diffuse reflectance and by

electrochemical impedance spectroscopy (EIS). Finally, the photocatalytic performance of the films was studied through discoloration of Methylene blue solution under visible radiation. Results showed that optical properties of the catalyst were enhanced after sensitization process. Furthermore, the IES results shows TiO_2/sensitizer system exhibited lower charge transfer resistance compared to bare TiO_2. Finally, the TiO_2/sensitizer system demonstrated photocatalytic activity under visible irradiation.

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Electrocleavage Synthesis of Molecular-Level Hybrid COF/Single-Layer MOF-Derivative MOOH Catalysts with Interface-Heterojunction for Biomass Electrooxidation Reaction

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Abstract:

A molecular-level hierarchical interface-heterojunction (IHJ) electrode of hybrid COF/single-layer MOF-derivative MOOH catalysis will be introduced. This system utilizes the complementary properties of COFs, which provide a porous scaffold with tunable chemistry, and MOF-derived MOOH, which offers abundant redox-active sites.[1] The hierarchical IHJ architecture promotes efficient charge separation and enhances electron/proton transport, significantly improving catalytic performance.[2] This will realize a synergistic multi-component design of biomass electrooxidation reaction (BEOR) catalysts from single to multi-scale, and will reveal the structure-component-performance relationships of hierarchical IHJ electrodes at multiple components.

Biography:

Lingling Wang is a Humboldt Research Fellow in the Fischer research group at the Technical University of Munich (TUM). Her research centers on the design and synthesis of covalent organic frameworks (COFs) and conjugated polymer networks. She has developed electrochemically driven solution-processing strategies for cross-linked conjugated polymers, enabling the controlled conversion of intrinsically insoluble materials from particulate states into uniform, device-compatible thin films. Her work addresses a critical bottleneck in processing robust π-conjugated systems and advances their integration into functional architectures. She is actively engaged in interdisciplinary research and international collaboration on advanced organic materials.

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Improving the Performance of Co/TiO_2 Catalysts by Mesostructuring the Support

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Abstract:

The effect of support mesoporous structuration has been studied for the Fischer-Tropsch synthesis reaction. One of the main drawbacks for this process is related to catalyst deactivation. Within this frame, reductive oxides such as TiO_2 also condition the final catalytic performance due to the occurrence of Strong Metal-Support Interaction (SMSI) effect. In this contribution, mesoporous titania supports were prepared by the surfactant templating pathway, using titanium isopropoxide, and the triblock copolymer P123 as structure-directing agent. The metallic phase was incorporated into the synthesized supports through the incipient wetness impregnation method. Commercial TiO_2 Evonik P90 has been used as reference material.

STEM/HAADF images of the obtained materials show Co nanoparticles well distributed along the mesopore channels of TiO_2. These well-ordered mesoporous Co/TiO_2, with the metal clusters located inside the mesopores, strongly affects the reducibility behaviour of cobalt, also improving the catalytic performance. Although the reduction pretreatment and reaction induce a drastic structural change of mesopores, the high catalytic performance is maintained.

Thus, we have demonstrated that porous structuration allows to stabilize the metal active sites and therefore to improve the catalytic performance. In that way, the confinement of Co particles within the pores hinders the strong metal–support interaction effect (SMSI), and highly stable metal active sites lead to better performance for Fischer–Tropsch synthesis reaction toward C5+ products.

Authors acknowledge the financial support through grant PID2020-119946RB-I00 and PID2024-160864OB-I00, funded by MCIN/AEI/ 10.13039/501100011033 and FSE+.

Biography:

My research activity has been focused on the development of catalytic systems with energy and environmental applications, with special emphasis on their physical and chemical characterization. Processes such as the elimination of NOx gases emitted in the combustion of explosion engines and those related to the production of hydrogen through reforming reactions, have been part of the main core of research. These works have been carried out mainly within the framework of research projects financed by the Spanish Ministry of Science, and others of international cooperation including European and international projects, as well as R+D+i contracts with different international companies.

Optimize the Chemical and Physical Properties of H-ZSM-5 Zeolite Catalysts to Produce Ethylene by the Process of Ethanol Dehydration

Makhosonke Ngcobo[1*], Thandeka Tshabalala[2], Johannes Ramothopo[2]

[1]University of South Africa, South Africa; [2]University of Johannesburg, South Africa

Abstract:

This research project was aimed at finetuning the physical and chemical properties of H-ZSM-5 using late transition metals to optimize the production of bioethylene from the bioethanol dehydration process. The metals that were loaded on the H-ZSM-5 catalyst are nickel and iron, in both monometallic and bimetallic forms. This is because iron improves the stability of the catalysts during ethanol dehydration, whilst nickel gives the best ethanol dehydration and ethylene selectivity. The solid acid catalysts, synthesized through hydrothermal and wet impregnation techniques, were characterized using PXRD, SEM-EDX, FTIR, BET, and TGA. The introduction of transition metals to the H-ZSM-5 affected the surface area, particle size, and elemental composition without altering the MFI structures of H-ZSM-5. The surface area of the catalysts was determined using BET to be between 289 and 418 $m^2 g^{-1}$. The FTIR and EDX confirmed the functional group and elemental composition, respectively. Notably, H-ZSM-5 constituted a higher affinity of iron (~7 %) than nickel (~5 %) metal atoms. TGA confirmed that the Ni/Fe-ZSM-5 bimetallic catalyst was the most stable, with only 2.71 % overall weight %

loss. The SEM images of the compounds revealed that the catalysts have irregularly shaped granules with rough surfaces. PXRD investigated the solid materials' phases, which showed characteristic peaks at 2θ = 21–25°, 32°, 45°, and 55°. The prepared materials served as good and stable catalysts for bioethanol dehydration to form bioethylene.

Biography:

Makhosonke Ngcobo is a senior researcher at the University of South Africa (UNISA) under the Institute of Catalysis and Energy Solutions (ICES). He received his PhD in 2021 from the University of KwaZulu-Natal. In 2022, he completed a postdoctoral fellowship at the University of the Western Cape, working on converting waste and residual biomass into bioenergy, biofuels, and bio-oils, followed by a postdoctoral fellowship at the University of Johannesburg in 2023. He is currently interested in the development of metal-based catalysts for the valorisation of biomass and CO_2.

POSTER PRESENTATIONS

Democratising the jellium model for plasmonic nanoparticles

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Abstract:

Plasmonic metal nanoparticles (NPs) convert (sun)light into hot carriers. These hot carriers can fuel chemical reactions through various mechanisms, depending on their energy, lifetime, and spatial distribution [1]. Modeling these mechanisms is frustrated by the size (tens of nm) of catalytically relevant NPs and the quantum nature of hot carriers [2]. The jellium model solves these issues by approximating the atomic structure of the NP by a homogeneous positive background charge [3]. In combination with Fermi's golden rule, one can compute the hot carrier population resulting from irradiation by light at a low computational cost. Furthermore, the jellium model can be straightforwardly expanded to describe e.g. the decay of hot carriers and charge transfer between a NP and an adsorbed molecule [4,5]. Owing to its theoretical simplicity, modularity, and low computational cost, the jellium model could 'democratise' theoretical analyses within the (experimental) plasmonic community and provide a starting point for more extensive theoretical approaches. Here, I provide an overview of recent use-cases of the jellium model, and share an illustrative open-source python implementation.

Biography:

Bibiana Türkcan is a PhD candidate at Leiden University, The Netherlands. With Dr. Jörg Meyer, she investigates how electronic excitations in metal surfaces can affect elementary reaction steps in heterogeneous catalysis. To this end, she develops and uses *ab initio* theoretical models. Bibiana graduated her Bsc (2022) at Leiden University and the Technical University of Delft *summa cum laude,* and her Msc (2025) at Leiden University, the Vrije Universiteit, and University of Amsterdam *cum laude*, in chemistry. During her Msc, she characterised the atomic structure of the Pd(111) electrode/electrolyte interface with *ab initio* molecular dynamics, and worked on modeling plasmonic catalysis.

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High-Entropy Metal Sulfides as Electrocatalysts for Overall Water Splitting

Elena Miliutina*, Vladislav Buravets, Vasilii Burtsev, Václav Švorčík and Oleksiy Lyutakov

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Abstract:

The development of efficient and low-cost electrocatalysts for water splitting is essential for sustainable hydrogen production and energy conversion. In this work, a simple method for the preparation of high-entropy sulfides (HES) based on Cr, Fe, Ni, Co, and Zn is presented. The synthesis uses common inorganic salts as precursors and CS_2 as a sulfur source. To obtain a homogeneous high-entropy composition, the precursor solution was frozen and freeze-dried before sulfurization. The sulfurization step was carried out in a flow reactor, and the final material was exfoliated in liquid nitrogen to obtain a 2D morphology. The structure and morphology of the prepared HES flakes were studied by TEM, HRTEM, AFM, XPS, XRF, SEM-EDX, and Raman spectroscopy, confirming successful synthesis of the target material. The electrocatalytic properties of the HES were tested in water splitting at different pH values. The as-prepared material showed moderate activity toward the hydrogen evolution reaction (HER). After electrochemical self-activation in acidic medium, HER performance increased significantly, especially in alkaline solution. In the oxygen evolution reaction (OER), the as-

prepared HES flakes showed good activity in alkaline medium even without pre-activation. The obtained results indicate that the prepared high-entropy sulfide is a promising bifunctional electrocatalyst for overall water splitting in alkaline media.

Biography:

Elena Miliutina received Ph.D. degree from UCT Prague in 2021. Over the past nine years, I have studied and worked at the University of Chemistry and Technology, Prague. My current research focuses on green energy technologies and supercapacitors based on 2D materials, addressing important societal, technological, and environmental challenges. My professional ambition is to develop innovative materials that contribute to a more sustainable future and improve quality of life. According to the Web of Science database, I am the author and co-author of 52 papers published in international journals, with more than 833 citations (without self-citations) and an H-index of 19.

Pt Nanoclusters on MXene for the Methanol Oxidation Reaction

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Affiliation: Department of Solid State Engineering, University of Chemistry and Technology, 166 28 Prague, Czech Republic

Abstract:

Two-dimensional materials of the MXene family attract considerable interest in electrochemical energy conversion due to their high electrical conductivity, large specific surface area, and rich surface chemistry. These properties make them promising supports for active sites in electrocatalysis. In this work, a catalytic material based on Mo2Ti2C3Tx MXene with electrochemically deposited Pt nanoclusters was investigated for the methanol oxidation reaction (MOR), which is of interest for direct methanol fuel cells. The Pt nanoclusters/Mo2Ti2C3Tx system was prepared by controlled cathodic polarization in sulfuric acid solution. Cyclic voltammetry data showed an increase in current density and a shift in the onset potential, indicating the formation of catalytically active sites. The obtained materials were characterized by XRD, Raman spectroscopy, UV-Vis, ICP-MS and AFM. XRD and Raman spectroscopy confirmed the successful synthesis of Mo2Ti2C3Tx from the parent MAX phase, while AFM confirmed the formation of thin layers with thicknesses of several nanometers. The combined ICP-MS and electrochemical data indicate the presence of Pt-containing redox-active sites on the MXene surface. Electrochemical characterization by CVA and CA demonstrated high activity of Pt nanoclusters/Mo2Ti2C3Tx toward methanol oxidation. In contrast to Pt-free control samples, the studied system exhibited pronounced oxidation peaks and high stability in alkaline media.

Biography:

Vasilii Burtsev, PhD is a researcher at UCT Prague specializing in Materials Engineering. He received degrees in Radiophysics and in Electronics and Nanoelectronics from Irkutsk State University and a PhD from UCT Prague, Czech Republic. His research interests include 2D materials, SERS, SEM-EDX, surface modification, and sensor development for the detection and monitoring of trace biologically active compounds. He is the first author and co-author of 38 international journal papers, with more than 455 citations, an H-index of 12, and two prototypes.

Continuous-Flow Plasmonic Catalysis: Insights Into Mass Transport Effects in Au@Pd Nanocatalysts During Suzuki Coupling

Mariia Erzina[1]*, Daria Votkina[2], Elena Miliutina[1], Malek Y. S. Ibrahim[3], Vaclav Svorcik[1], Markus Valtiner[4], Oleksiy Lyutakova[1], Olga Guselnikova[4]

[1]University of Chemistry and Technology, Prague, Czech Republic; [2]Research School of Chemistry and Applied Biomedical Sciences, Tomsk, Russian Federation; [3]Redeem Solar Technologies GmbH, Graz, Austria; [4]Vienna University of Technology, Vienna, Austria

Abstract:

Plasmonic catalysis represents a promising approach for driving chemical transformations using solar energy. However, most reported systems operate in millilitre-scale batch reactors with milligram quantities of nanocatalysts, limiting their practical applicability in standard laboratory and industrial settings. A transition to continuous-flow systems is therefore required, yet the interplay between plasmon-induced processes and mass transport remains insufficiently understood. In this work, a flow-based plasmonic catalytic platform operating at the tens-of-millilitres scale using gram-scale Au@Pd nanoparticle–Al_2O_3 composites was developed. The Suzuki cross-coupling reaction was selected as a model to evaluate system performance. Compared to batch conditions, the flow configuration significantly enhances reaction efficiency, leading to faster conversion, reduced reaction time, and a threefold increase in apparent quantum yield. Computational fluid dynamics simulations reveal that the residence time of catalyst–reactant complexes under illumination plays a decisive role in determining product yield. These findings are supported by photocurrent measurements, which indicate improved electron transfer efficiency under enhanced mass transport conditions. In contrast to prior studies focusing mainly on charge carrier behaviour within plasmonic heterostructures in static systems, our results demonstrate that effective transfer of charge carriers to reactants is a key factor governing catalytic performance under flow conditions. Overall, this study establishes a conceptual and practical basis for implementing

plasmonic catalysis in continuous-flow systems and provides guidelines for designing scalable light-driven chemical processes.

Biography:

Mariia Erzina, Ph.D., is an interdisciplinary researcher specializing in surface-enhanced Raman spectroscopy (SERS), with 23 Web of Science–indexed publications, 416 citations, and an h-index of 11. Her work focuses on the design of plasmonic nanostructures for applications in detection, photocatalysis, and photoelectrocatalysis. She integrates SERS with machine learning to enable predictive understanding of analyte–substrate interactions. Dr. Erzina has strong expertise in Raman and UV–vis spectroscopy and in correlating nanostructure morphology, surface chemistry, and plasmonic properties with SERS signal enhancement and reproducibility.

Efficient Electrochemical CO_2 Reduction to Ethylene on Thermal-Reduced Copper Electrodes

Xianyun Zhang[1]*, Haining Tian[1]

[1]*Uppsala University, Sweden*

Abstract:

Electrochemical CO_2 reduction (ECO_2R) to multicarbon (C2+) products in neutral electrolytes represents a promising route toward carbon neutrality. Oxide-/hydroxide-derived Cu catalysts have demonstrated enhanced selectivity toward C2+ products; however, rational design strategies to further improve performance remain limited. Here, we report a CO-atmosphere thermal reduction strategy to fabricate a high-performance Cu-based electrode (CO-Cu) from $Cu(OH)_2$ precursors. Fourier-transform infrared spectroscopy (FTIR) confirmed complete removal of residual CO from the catalyst surface. The electrochemical active surface area (ECSA), determined via electrochemical double-layer capacitance measurements, was 60-fold greater than that of polished Cu, indicating a substantially enlarged catalytic interface. In situ Raman spectroscopy further revealed that CO-Cu facilitates high surface coverage of *CO intermediates under moderate applied potentials, thereby promoting C–C coupling pathways toward C2+ products. Consequently, CO-Cu achieved a total C2+ Faradaic efficiency exceeding 60%, with ethylene selectivity maintained above 40% over 37 hours of continuous operation, demonstrating both high activity and long-term stability.

Biography:

Dr. Xianyun Zhang received his PhD in Materials Physics and Chemistry from the University of Chinese Academy of Sciences in 2021 and is currently a Postdoctoral Researcher at Uppsala University. His research background spans electrochemistry and additive manufacturing, with a current focus on electrochemical CO_2 reduction. He has expertise in operando Raman spectroscopy for probing dynamic surface processes and reaction pathways during catalysis. His work aims to advance carbon conversion technologies and enable the rational design of high-performance catalysts and electrochemical reactors.

Enzymatic Biocatalysis as a Sustainable Route to Bio-Adhesives from Agro-Food Residues

Aušra Šimonėlienė[1], Vilma Šipailaitė-Ramoškienė[2], Tomas Makaveckas[3]

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[2] Centre for Engineering Studies, Faculty of Informatics, Engineering and Technologies, Kauno kolegija, Pramonės pr. 22, Kaunas, LT-51189.
[3] Alytus Faculty, Kauno kolegija, Studentų g. 17, Alytus, LT-62252

Abstract:

The growing demand for sustainable materials has increased interest in lignocellulosic biomass valorization. Agro-food residues are abundant renewable resources that can be converted into valuable chemicals and bio-based products. Lignin, a primary component of lignocellulosic biomass along with cellulose and hemicellulose, has emerged as a promising raw material for bio-adhesives, polymers, and other functional materials.

Traditionally, lignin has been considered a low-value by-product and is often burned for energy. Its aromatic structure allows it to act as a natural phenolic polymer, partially replacing synthetic phenol in adhesive formulations. Conventional chemical extraction methods often modify lignin's structure and are not environmentally sustainable. In contrast, biocatalysis approaches using cellulase selectively hydrolyze cellulose, releasing lignin-rich fractions while largely preserving lignin's native structure.

This study investigated enzymatic biocatalysis for lignin isolation from selected agro-food residues and its potential for bio-adhesive production. Five residues were studied: cereal straw, buckwheat husks, coffee bean husks, walnut shells, brewery plant residues. Samples were dried, milled to increase surface area; mildly pretreated to enhance enzyme accessibility. Cellulase enzymes degraded cellulose into soluble sugars, leaving lignin-enriched solid fractions.

Results showed that cereal straw, coffee bean husks, brewery residues were more easily hydrolyzed, whereas walnut shells and buckwheat husks resisted hydrolysis due to their dense lignified structure. Processing cereal straw and coffee husks yielded lignin concentrations 3–4 times higher. These findings confirm that biocatalysis is an effective and promising strategy, enabling sustainable bio-adhesive production from agro-food residues while maintaining lignin's native structure and improving raw material functionality for industrial applications.

Biography:

PhD. Aušra Šimonėlienė works in the field of food fermentation technologies, focusing on sustainable production, efficient utilization of raw materials and resources, and the development of biotechnological processes for industrial applications. PhD. Vilma Šipailaitė-Ramoškienė and PhD. Tomas Makaveckas specialize in materials engineering, studying the design, optimization, and industrial application of novel materials, including sustainable polymers. All researchers have extensive experience, have participated in international projects and publications, and have contributed to the development of innovative solutions in their respective fields.

Assessment of Lignocellulosic Feedstocks for Efficient Bioenergy Catalytic Conversion Technologies

Tetiana Kulik[1,2]*, Borys Palianytsia[1], Vita Halysh[1,3]

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[1]Chuiko Institute of Surface Chemistry, NAS of Ukraine, Ukraine;
[3]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Ukraine

Abstract:
The shift toward a circular bioeconomy relies heavily on the integration of lignocellulosic biomass as a primary carbon source for sustainable energy [1]. However, the technical feasibility of various catalytic conversion pathways is fundamentally dictated by the plant's internal structure - specifically the distribution of cellulose, hemicellulose, lignin, and inorganic residues. This research investigates the chemical profiles of winter wheat straw, miscanthus, and willow to establish a data-driven framework for matching specific feedstocks with optimal processing technologies.

Analytical results indicate that wheat straw and miscanthus are particularly rich in polysaccharides, with cellulose levels reaching 44.2% and 43.5% respectively. This high carbohydrate density suggests these materials are ideal candidates for enzymatic

saccharification and subsequent biochemical refining. Conversely, willow exhibits a lower cellulose concentration of 38.9% but excels in thermochemical stability. A critical differentiator is the ash concentration, which peaks in wheat straw at 6.4% and drops to a negligible 0.9% in willow. This disparity is vital for industrial scaling, as low-ash materials like willow significantly reduce the risk of reactor fouling and slagging during high-temperature combustion. The study further highlights the complex solubility of wheat straw, which contains 36.7% NaOH-soluble and 9.9% hot water-soluble fractions, necessitating specialized pre-treatment protocols. Ultimately, while wheat straw offers high yields for liquid biofuels, willow remains the superior choice for direct thermal energy recovery. Miscanthus occupies a flexible middle ground, proving effective across multiple platforms.

These findings underscore that maximizing bioenergy sustainability requires a tailored approach where the choice of catalytic conversion technology is directly informed by the raw material's unique chemical properties.

1. Halysh, V., Romero-García, J. M., Vidal, A. M., Kulik, T., Palianytsia, B., García, M., & Castro, E. (2023). Apricot seed shells and walnut shells as unconventional sugars and lignin sources. Molecules, 28(3), 1455.

Acknowledgments:

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Valorization of Cocoa Pod Husk *via* Chemical Modification and Pyrolysis toward Catalytic Applications

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Abstract:

The development of efficient strategies for the fractionation and valorization of lignocellulosic biomass from agricultural and food industry waste is essential for advancing green technologies toward the production of biofuels and value-added chemicals. In this work, cocoa pod husk waste was used as a model feedstock to demonstrate the effectiveness of sequential acid–alkaline treatment and chemical modification, including phosphorylation, sulfuration, carboxylation, oxidation, carbonization, and activation, for the preparation of functional lignocellulosic materials.

The structural features and chemical properties of cellulose and lignin were elucidated using a complex of physicochemical techniques, including solid-state ^{13}C NMR, FTIR, TPD-MS, MALDI-TOF MS, SEM, and adsorption–desorption analysis. The isolated lignin was shown to differ from typical guaiacyl–syringyl lignins due to the presence of additional *p*-coumaric units. Pyrolysis studies of raw biomass and fractionated materials revealed distinct thermal transformation stages of hemicellulose, cellulose, and lignin. Sequential treatment enabled efficient hemicellulose removal and selective isolation of lignin- and cellulose-rich fractions, facilitating their targeted valorization. Lignin-derived materials can serve as precursors for polyphenolic building blocks, advanced polymers, and functional additives, while cellulose-derived fractions yield furan-based compounds. Carbonized materials and biochar exhibit potential as sorbents and catalyst supports.

Overall, this study highlights the potential of integrated green processing and catalytic strategies for the efficient valorization of lignocellulosic waste into high-value chemicals and functional materials, contributing to the development of sustainable and circular bio-based technologies.

Biography:

Dr. Alina Nikolaichuk is a Senior Researcher in the Laboratory of Kinetics and Mechanisms of Chemical Transformations on Solid Surface, Chuiko Institute of Surface Chemistry of the NAS of Ukraine. She received her Ph.D. in Physical Chemistry in 2021. Her research interests include the investigation of various pretreatment, modification, and separation methods for lignocellulosic biomass from agricultural waste into its individual components to obtain value-added products for various applications. She conducted her postdoctoral research at KTH Royal Institute of Technology and at Uppsala University, Sweden.

Transfer Reductive Mechanochemical Upcycling of Polyethylene

Antonio Cosimo Pio Trimboli[1]*, Emilia Paone[1], Andrea Donato[1], Riccardo Pellegrini[2], Elena Groppo[3], Maximilian Wohlgemuth[4], Sven Grätz[4], Lars Borchardt[4], Francesco Mauriello[1]

[1]*Università degli Studi Mediterranea di Reggio Calabria, Italy;* [2]*Chimet S.p.A., Italy;*
[3]*Università degli Studi di Torino, Italy;* [4]*Ruhr-Universität Bochum, Germany.*

Abstract:

Plastic production has increased dramatically over the last decades and now exceeds 400 million tonnes per year, with polyolefins representing the largest share of both produced plastics and accumulated waste. Despite growing efforts to develop circular solutions, most post-consumer polyolefins are still incinerated or landfilled, highlighting the limitations of current recycling technologies. Mechanical recycling often results in materials with downgraded properties, while chemical recycling typically requires high temperatures or pressurized hydrogen, leading to energy-intensive processes.[1] Here we present a mechanocatalytic strategy for the upcycling of polyethylene that combines mechanical activation with catalytic transfer hydrogenation. The system employs a commercial Ru/Al_2O_3 catalyst with hydrogen-donor alcohols, enabling polymer depolymerization under ambient conditions without the use of molecular hydrogen. Among the alcohols investigated, 2-propanol proved to be the most effective, acting both as hydrogen donor and liquid-assisted grinding agent. Four mechanochemical platforms, mixer mill, planetary mill, vibratory disc mill, and resonant acoustic mixer, were systematically evaluated to assess the influence of mechanical activation. Under optimized conditions, the mixer mill delivered the best performance, achieving 30% polyethylene conversion after 6 h and producing predominantly liquid hydrocarbons, with more than 95% of products in the C5-C20 range and negligible gas formation.[2] The methodology was successfully extended to ultra-high molecular weight polyethylene and real post-consumer polyethylene waste.

[1] J. Sun, J. Dong, L. Gao, Y.-Q. Zhao, H. Moon, and S. L. Scott, Chem.Rev., 2024,124, 9457−9579.

[2] A. C. P. Trimboli, E. Paone, A. Donato, R. Pellegrini, E. Groppo, S. Graetz, F. Mauriello, *ChemRxiv., 2025, doi:10.26434/chemrxiv-2025-7tck7*

Biography:

Antonio Cosimo Pio Trimboli is a PhD student at the University of Reggio Calabria (UniRC), where his research focuses on the catalytic recycling of polyolefin plastics. He obtained his bachelor's degree in Industrial Engineering in 2021 and his master's degree in Energy and Nuclear Engineering in 2023 from the same institution. He is currently a visiting PhD student at Ruhr University Bochum, where he is working on the mechanocatalytic valorization of polyolefins.

Upcycling of Coconut Shell into Bifunctional Sulfonated Catalysts for Enhanced Sugar Hydrolysis

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2Departamento of Engineering, University of Messina, Messina, Italy.

3Departamento de Procesos Químicos, Alimentos y Biotecnología, Facultad de Ingenierías y Ciencias Aplicadas, Universidad Técnica de Manabí, Portoviejo, 130101, Ecuador.

Abstract:

This work reports the valorization of coconut shell waste into bifunctional sulfonated carbon catalysts bearing Lewis and Brønsted acid sites for the production of high-value furanic compounds. Catalysts were prepared via $ZnCl_2$ activation followed by H_2SO_4 sulfonation to enhance acidic site distribution and synergy. Their performance was evaluated in the conversion of xylose to furfural (FF) and glucose/fructose to 5-HMF under varying reaction conditions. The $ZnCl_2$-AC_{500}-S catalyst showed superior activity, achieving 87.3% FF yield from xylose and up to 98.2% 5-HMF from fructose. The results demonstrate a synergistic interplay between Lewis sites (isomerization) and Brønsted sites (dehydration). These findings highlight coconut shell as a sustainable precursor for efficient, reusable catalysts in biomass upcycling.

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Chheda, J. N.; Román-Leshkov, Y.; Dumesic, J. A. Production of 5-hydroxymethylfurfural and furfural by dehydration of biomass-derived mono- and poly-saccharides. Green Chemistry, 2007, 9, 342–350.

Sudarsanam, P.; Peeters, E.; Makshina, E. V.; Parvulescu, V. I.; Sels, B. F. Functionalised heterogeneous catalysts for sustainable biomass valorisation. Chemical Society Reviews, 2019, 48, 2366–2421.

Cascade Biorefinery Strategy for the Valorization of Orange Peel Waste into Bioactive Compounds, Sugars, and Biomethane

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[b] *Dipartimento di Ingegneria Civile, Energia, Ambiente eMateriali (DICEAM), Università degli Stdi*

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Abstract:

Orange processing generates large amounts of peel waste, highly moist and rapidly degradable, which can cause odor, greenhouse gas emissions, and disposal costs if unmanaged. However, these residues contain valuable bioactive compounds and carbohydrates[1]. This study proposes a cascade biorefinery approach to convert orange peel waste into multiple products. Phenolic compounds are first extracted, yielding antioxidant-rich fractions. The remaining biomass undergoes acid hydrolysis to release fermentable sugars for biofuels or biobased chemicals[2]. Hydrolysis residues are treated via anaerobic digestion to produce biomethane, while the digestate serves as a nutrient-rich soil amendment[3]. This integrated process demonstrates a sustainable strategy for valorizing orange peel waste and supports circular bioeconomy principles.

[1] De la Torre, I., Martin-Dominguez, V., Acedos, M.G. et al. Appl Microbiol Biotechnol 103, 5975–5991 (2019). https://doi.org/10.1007/s00253-019-09929-2 [2]Balu, Alina Mariana, et al. "Valorisation of orange peel residues: waste to biochemicals and nanoporous materials." ChemSusChem 5.9 (2012): 1694. DOI: 10.1002/cssc.201200381 [3]Paolo S. Calabrò, Maria F. Panzera,Thermal Science and Engineering Progress, Volume 6, 2018, Pages 355-360, ISSN 2451- 9049, https://doi.org/10.1016/j.tsep.2017.12.011

Biography:

Silvia Sorbo holds a degree in Chemistry and Pharmaceutical Technology from the University of Messina, Italy, with a thesis in pharmacotherapy. She is a PhD candidate at the Department of Engineering, University of Messina, researching green chemistry and circular economy strategies. Her work focuses on valorizing agro-industrial residues, including lignocellulosic fractions of orange peel waste, to produce bioactive compounds.

Direct Valorization of Spent Lithium-Ion Batteries: Layered-to-Spinel Structural Transformation for Catalytic Applications

Giulia Maria Itri*1, Tapio Salmi3, Andrea Donato1, Adriana Pietropaolo2, Pierrafaele Barretta2, Chiara Alessandrello1, Claudia Triolo1, Francesco Mauriello1, Emilia Paone1

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3 Laboratory of Industrial Chemistry and Reaction Engineering (TKR)), Åbo Akademi University, Turku/Åbo, Finland

Abstract:

The increasing diffusion of spent lithium-ion batteries represents a significant environmental challenge; however, their active materials offer promising opportunities for catalytic reuse. In this work, a cobalt-based catalytic material was obtained from $LiCoO_2$ cathodes recovered from end-of-life batteries through a simple mechanical treatment followed by thermal activation. The thermal treatment was applied to remove residual organic binders and promote a structural rearrangement of the cobalt oxide framework.

The physicochemical properties of the materials were investigated using several characterization techniques, showing that the pristine material retains the typical layered structure of $LiCoO_2$, whereas calcination promotes a partial structural transformation toward a spinel-type cobalt oxide phase. The catalytic performance of the obtained materials was evaluated in the hydrogenation of furfural, an important biomass-derived platform molecule, both in the presence of molecular hydrogen and under catalytic transfer hydrogenation conditions. The catalyst exhibits high selectivity toward furfuryl alcohol at short reaction times, while longer reaction times favour the formation of the secondary hydrogenation product, tetrahydrofurfuryl alcohol (THFA). Complementary computational calculations further indicate that spinel-type $LiCoO_2$ surfaces provide more favorable adsorption interactions for furfural compared to the layered structure, providing an atomistic explanation for the observed catalytic behavior.

Overall, these results demonstrate the potential of materials derived from spent LCO batteries as sustainable catalysts for biomass valorization processes.

Biography:

Giulia Maria Itri holds a master's degree in chemistry and is currently a PhD candidate in the National PhD Program in Catalysis (39th cycle). Her research focuses on green chemistry and circular economy strategies, particularly the valorization of waste-derived materials, such as spent lithium-ion batteries and electronic waste, to develop heterogeneous catalysts for sustainable chemical production.

Sustainable Valorization of Sodium Aluminate Waste for Environmental and Catalytic Applications: ALTEREGO Project

Chiara Alessandrello1*, Francesco Mauriello 1, Emilia Paone1, Raffaele Cucciniello2, Michele Sisani3

1Università degli Studi Mediterranea di Reggio Calabria, Italy; 2Università di Salerno, Italy; 3Prolabin&Tefarm S.r.l., Italy

Abstract:

The ALTEREGO project focuses on the development of innovative valorization strategies for sodium aluminate waste (SAW), a by-product generated during the alkaline surface treatment of aluminum profiles. The project aligns with the principles of circular economy and industrial symbiosis by promoting resource recovery, waste minimization and a consequential reduction in the environmental impact.

The main objective is the recovery of aluminum from SAW in the form of aluminum hydroxide (Al(OH)3), which will serve as a precursor for the synthesis of hydrotalcites and layered double hydroxides (LDHs), including environmentally friendly doped systems such as Fe-containing materials. A particular attention will be devoted to tuning the acid-base properties and interlayer anions of the prepared materials with the aim of optimizing their catalytic and adsorption performances.

The developed materials will be applied in three main areas: heterogeneous catalysis for the synthesis of cyclic organic carbonates through the cycloaddition of CO2 to epoxides, adsorption and degradation of surfactants from wastewater via advanced oxidation processes, including Fenton and photo-Fenton reactions and arsenic removal from drinking water.

To assess the environmental sustainability of the proposed processes, the project will also include a Life Cycle Assessment (LCA) study aimed at quantifying the benefits associated with green chemistry approaches and evaluating the potential industrial scale-up of the developed technologies.

Biography:

Graduated in Chemistry in 2020, she obtained a PhD in Chemical Sciences with a thesis focused on the physicochemical characterization of landfill leachate and on the investigation of its complexing properties toward metal cations. She is currently a research fellow at the Università degli Studi Mediterranea di Reggio Calabria, where she is involved in the ALTEREGO project. Her current research activity focuses on the valorization of sodium aluminate waste through the synthesis of functional hydrotalcites and layered double hydroxides for catalytic applications.

Enhanced Catalytic Performance of Phosphorus-Modified Zeolite Nano-Sheets Synthesized via DABCO-Based Surfactants

Sara Karimi1*

1Allameh Tabarsi University, Babol, Iran

Abstract:

Zeolite ZSM-5 nano-sheets with a plane morphology were synthesized using DABCO-based cationic surfactants through a hydrothermal route. The effects of surfactant structure, synthesis ratios, and phosphorus modification on morphology and catalytic activity were investigated. The products were characterized using SEM, TEM, XRD, BET, and FTIR analyses. Chemometric tools (MCR-ALS) were applied to interpret DRIFT spectra and monitor synthesis evolution. Results revealed that minimizing the SiO_2/Al_2O_3 ratio while maximizing template/SiO_2 and H_2O/SiO_2 ratios led to the thinnest layer morphology (≈5.5–10 nm). The phosphorus-modified nano-sheets exhibited enhanced surface acidity and improved catalytic performance, indicating their potential for petrochemical applications.

Keywords: Zeolite nano-sheets, DABCO surfactant, phosphorus modification, chemometrics, spectroscopy

Biography:

Sara Karimi holds a B.Sc. in Chemical Engineering from Allameh Tabarsi University, Babol, Iran. She has professional experience as a technical and quality control officer at the Khorasan Petrochemical Laboratory in Bojnord. Sara has also participated in advanced courses and research programs in Budapest, Hungary. Her research interests include catalysis, nanostructured zeolites, and green chemical engineering. She has contributed to several projects and presented her work at conferences on catalysis and materials science, with plans for publication in international journals.

DAY-3, JULY 01, 2026

Keynote Talks

Recent Advances in Palladium Iodide Catalyzed Carbonylative Transformations

Bartolo Gabriele*

University of Calabria,Italy

Biography:

Bartolo Gabriele was born in Cosenza, Calabria (Southern Italy). He received the degree in Chemistry (1990) and completed his PhD in Chemical Sciences (1994) at the University of

Calabria. After a post-doc experience at Columbia University (New York) with Prof. Ronald Breslow (1997-1998), he returned to the University of Calabria, where he was promoted to Associate Professor in 2002 and to Full Professor of Organic Chemistry in 2006. Prof. Gabriele has published so far 269 papers in peer-reviewed journals, 21 chapters in international books, is the co-inventor of 20 patents (12 national, 8 international). In 2022, he edited the book *Carbon Monoxide in Organic Synthesis – Carbonylation Chemistry* with Wiley. Prof. Gabriele received the award in Synthetic Organic Chemistry from the Organic Chemistry Division of the Italian Chemical Society in 2013 and the Senior award in Organometallic Chemistry from the Interdivisional Group of Organometallic Chemistry of the Italian Chemical Society in 2024.

NiGraf and Reduced NiGraf: A New Family of Catalytic Metal Organic Alloys of Large Applicative Potential

Mario Pagliaro[1]*, Matteo Formenti,[2] Rosaria Ciriminna,[1] Cristina Della Pina [2]

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Abstract:

Consisting of graphene oxide molecularly entrapped within jamborite nanoparticles, NiGraf (GO@Ni) is a new metal-organic alloy (MORAL) usable as versatile electrocatalyst for both hydrogen and oxygen evolution reactions in alkaline water electrolysis. Its reduced form obtained via reduction of entrapped GO with thiophene (RGO@Ni) is a highly active and stable hydrogenation catalyst enabling the reduction of nitrobenzene (NB) to aniline at 35 °C in the liquid phase using water as an “on-solvent” reaction medium under biphasic conditions. In this presentation, I will discuss the outcomes of experimental and computational investigations of both NiGraf and reduced NiGraf explaining the unique catalytic activity and stability of these new MORALs. Applications range from use of reduced NiGraf in mediating the nitrobenzene hydrogenation to aniline through successful employment of NiGraf in the electrocatalytic oxygen evolution reaction (OER), which is usually the most sluggish half-reaction in alkaline water electrolysis due to the multi-electron transfer process. These results are practically relevant because MORALs hold great applicative potential as new-generation solid catalysts, especially when the metal used to entrap organic species consists of low-cost and earth-abundant nickel. For instance, besides eliminating the need for an organic solvent, the reduction of NB to aniline at room temperature mediated by reduced NiGraf has significant practical application potential for the synthesis of a compound produced worldwide at a rate of 7 million tonnes per year.

Biography:

Research Director at Italy's National Research Council Mario Pagliaro leads in Palermo, Italy, a research Group working in a broad field encompassing biochemistry, nanochemistry, solar energy, green chemistry, and the bioeconomy. In 2021 he was elected ordinary member of the Academia Europaea. “IntegroPectin”, "CuproGraf", “NiGraf”, “CytroCell”, “GrafeoPlad”, “CytroCav”, “AquaSun”, “SiliOrange”, “AnchoisOil”, “Omeg@Silica”, “LimoFish”, "AetnAsh", “AnchoisFert”, “SiliaSun”, “TitaniaSun”, and “HyTan” are some of the names created by Dr Pagliaro to identify new functional materials and new enabling technologies jointly developed by his Lab. All his team’s papers are openly accessible being self-archived on his personal academic website (qualitas1998.net).

Waste Valorization into Chemicals and Fuels Using Nanocatalysis

Sudarsanam Putla*

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Abstract:

Valorization of plastic waste and non-edible lignocellulosic biomass into chemicals and fuels is a promising strategy to reduce fossil-fuel dependence and net carbon emissions [1-10]. Both plastic and biomass consist of rigid carbon-rich polymer structures with strong C–C and C–heteroatom bonds, which makes their conversion under mild conditions challenging. Heterogeneous catalysis using metal and metal oxide nanomaterials offers cost-effective routes for transforming plastic and biomass into valuable products. Tuning the size and shape of metal/metal oxide nanoparticles offers highly active surface acid–base and redox properties, with selective performance. In this talk, I will discuss the fundamentals and catalytic applications of metal and metal oxide nanocatalysts for (i) valorization of PET plastic waste into value-added monomers and (ii) converting lignocellulosic biomass-derived furans into chemicals and fuel precursors.

Keywords: Waste-to-value; plastic waste recycling; biomass conversion; nanocatalysis; sustainable processes

Biography:

Dr. Sudarsanam Putla is an Assistant Professor at the Department of Chemistry, IIT Hyderabad (IITH), India. Before joining IITH (April 2022), he was a Scientist at CSIR-National Chemical Laboratory, Pune (Feb 2020- March 2022). He obtained his Ph.D. degree in Chemistry (2014) from CSIR-IICT, Hyderabad. From 2014 to 2019, he worked as a postdoctoral fellow at RMIT

University (Melbourne), Leibniz Institute of Catalysis (Germany), and KU Leuven (Belgium). His research group primarily works in Heterogeneous Catalysis, focusing on the development of advanced catalytic materials and sustainable catalytic processes for plastic waste recycling and biomass valorization. He has received several awards/fellowships: RSC Nanoscale Emerging Investigator-2025, PECFAR Award-2024 (Indo-German Science & Technology Centre), Young Scientist Award-2024 (Catalysis Society of India), Associate Fellow of the Telangana Academy of Sciences-2024, Australian Alumni Award-2021, Marie-Curie Fellowship-2017, Leibniz-DAAD Fellowship-2017, Best PhD Thesis Award-2015 (Catalysis Society of India), and Endeavour Research Fellowship-2013 (Australia). He has authored over 100 publications in high-impact peer-reviewed journals (h-index: 43, with ~6,700 citations), five book chapters, edited 4 books, and serves on Advisory/Earle Career Editorial Boards of various peer-reviewed journals, including RSC Sustainable Energy & Fuels, ACS Sustainable Chemistry & Engineering, Molecular Catalysis, and Applied Catalysis O: Open.

Unconventional Solvents: A Powerful Reaction Media for Heterocyclization Processes

Raffaella Mancuso*

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Abstract:

Heterocyclization reactions, represent a cornerstone of modern synthetic chemistry, enabling the efficient construction of heterocycles, a class of structures widely present in pharmaceuticals, natural products, and functional materials. Among the various heterocyclization strategies, iodocyclization has emerged as a powerful and versatile method that exploits the high electrophilicity and leaving-group ability of iodine reagents to promote intramolecular carbon-heteroatom bond formation. Iodocyclization reactions typically proceed under mild conditions and often provide excellent regio- and stereoselectivity, making them attractive for the synthesis of oxygen-, nitrogen-, and sulfur-containing rings. Unconventional solvents, on the other hands, such as ionic liquids (ILs) and deep eutectic solvents (DESs), are emerging as valuable alternatives to traditional volatile organic solvents. Their distinctive physicochemical characteristics, including tunable polarity, enhanced thermal and chemical stability, low vapor pressure, and the ability to form highly structured solvation environments, offer unique advantages for chemical synthesis, extraction, catalysis, and materials processing. Unconventional solvents not only improve reaction efficiency and selectivity but also contribute to the principles of green chemistry by reducing environmental impact and enabling more sustainable processes. In this communication, I will show as

unconventional solvents can significantly enhance both Metal-catalyzed heterocyclization and iodocyclization reactions. In Matal-catalyzed heterocyclization processes, these media can first of all promote intramolecular bond forming steps by facilitating favorable solute-solvent interactions and then offer the possibility of recycling the metal catalyst several times without loss of catalytic efficiency. Similarly, in iodocyclization reactions, unconventional solvents can boost the electrophilicity of iodine-based reagents and support highly controlled cyclization pathways.

Biography:

Prof. Raffaella Mancuso is a Full Professor of Organic Chemistry at the University of Calabria. He completed his degree (2002) and PhD (2006) at the same university. In 2008 she was a post-doc researcher at the Iowa State University (USA) and in 2012 an invited researcher at the University of Barcelona-Spain. In 2018 she was Researcher in Organic Chemistry and in 2021 Associate Professor. Her current scientific production include 180 papers, 8 patents, 9 book chapter and 280 communications in conferences. Her current research interests include organometallic catalysis for the synthesis of high value molecules, use of nonconventional solvents, and synthesis of novel materials for advanced applications.

Invited Talks

Catalytic Oxidative Desulphurization of Pyrolytic Oils to Fuels Over Different Waste Derived Carbon-Based Catalysts

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Abstract:

Oil recovered from pyrolysis of tires is a very attractive product stream due to their composition that is very close to an engine fuel [1]. Nonetheless, their sulphur content is generally very high avoiding their for real field applications and requires an upgrading process to met the fuel regulation requires.Considering the required desulphurization thrust and the

high content of refractory sulfur compounds, the most suitable technique is oxidation. This technique oxidizes sulphur compounds into sulphons, which are characterized by a more marked solubility towards polar solvents. We run oxidation a biphasic catalytic system in which the oxidizing agent (H_2O_2) performing a quasi-Fenton reaction catalyzed by iron tailored carbon materials recovered from pyrolysis of tires and coffee [2]. The Fe (III) of the catalytic species is generated by passivation of the Fe nanoparticles deposited through the carbothermal process. The characterization confirmed the formation of Fe nanoparticles with a hemispherical configuration whose external layer is composed of Fe oxides. The eccentricity of the catalytic surface caused a stress on the crystalline lattice of Fe oxide with an electronic distribution which allowed to obtain a high reactive system. The ICP results confirmed the reactivity of the system which achieved efficiencies between 35% and 60% under different operating conditions.

References:

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Designing Ru Catalysts from Atomic to Nanoparticle Scale: Mechanistic Insights from Multiscale Modeling

Hsin-Yi Tiffany Chen[1-3]*

1Department of Engineering & System Science; 2Department of Materials Science & Engineering; 3College of Semiconductor Research, National Tsing Hua University, Hsinchu 300044, Taiwan

Abstract:

Designing next-generation Ru-based catalysts for mild-condition ammonia conversion can unleash the potential of ammonia as an efficient renewable energy carrier. Currently, Ru-based catalysts suffer from high cost and hydrogen poisoning, which is addressed by controlling the size and dispersion of Ru species. Here, we have employed multiscale modeling, integrating density functional theory (DFT) calculations with ab initio molecular dynamics (AIMD) and deep potential molecular dynamics (DPMD) simulations to analyze catalysts from atomic to nanoparticle scales, providing in-depth mechanistic understanding of how to optimize Ru-based catalysts for ammonia production and decomposition. Our DFT

calculations revealed that Ru SACs on MgO(111) form multiple Ru-O pairs that facilitate heterolytic cleavage of hydrogen [1] or ammonia [2] and drive subsequent hydrogen spillover, suppressing hydrogen poisoning and enhancing catalytic ammonia conversion activity. This highlights the impact of supports at the atomic scale. When considering Ru8 cluster models, the importance of Ru B5 site geometry emerges, facilitating enhanced orbital coupling with and activation of N2.[3] Extending to nanoparticle scales, DPMD simulations show how Ru nanoparticle morphology changes with size.[4] Moreover, low-coordination sites on Ru nanoparticles can adsorb multiple hydrogen species, leading to nonlinear scaling between metal size and hydrogen adsorption capacity.[5] Altogether, these studies provide a fresh big-picture perspective into the different catalyst behaviors and reaction mechanisms that dominate at different size scales of Ru catalysts for ammonia conversion. These insights are expected to guide the future design of Ru-based catalysts for sustainable ammonia production and decomposition.

Biography:

Professor Hsin-Yi Tiffany Chen completed her PhD from the University College London under the mentorship of Professor Richard Catlow. She then conducted postdoctoral research at the University of Milano-Bicocca, under Professor Gianfranco Pacchioni. She became a professor at the National Tsing Hua University in 2016 and established the Energy Materials Modeling Group. Her work integrates first-principles calculations with machine-learning-based multiscale methods to advance research in catalysis, energy storage, semiconductors, and complex alloy systems. The impact of her research contributions as a young scientist has earned her awards from her university and multiple research societies.

Reframing the Amazon: From Biodiversity Reservoir to a Global Platform for Catalysis Biorefineries, and Sustainable Innovation

Luís Adriano Santos do Nascimento*[1], Ana Alice Farias da Costa[1], Maitê Thaís Barros Campos[1], Rutiléia de Jesus Paiva[1], Vanessa Albuquerque de Mescouto[1], Alex de Nazaré de Oliveira[2], Carlos Emmerson Ferreira da Costa[3], Geraldo Narciso da Rocha Filho[3] and Renata Coelho Rodrigues Noronha[1]

[1]Federal University of Pará/Graduation Program in Biotechnology, Brazil)

[2]Federal University of Amapá/ Department of Exact and Technologic Sciences, Brazil

[3]Federal University of Pará/Graduation Program in Chemistry, Brazil)

Abstract:

Over the past 15 years, the Catalysis and Oleochemistry Research Group at the Federal University of Pará (UFPA), in the Brazilian Amazon, has advanced a research agenda that positions the region not only as a source of biodiversity, but as a generator of high-level scientific knowledge and innovation. This work is driven primarily by researchers born and trained in the Amazon, combining territorial expertise with an expanding international scientific presence.

Our research integrates catalysis, green chemistry, and biotechnology to convert regional biomass—such as agro-industrial residues, mining by-products, vegetable oils, and lignocellulosic materials—into high-value products, including biofuels, fine chemicals (e.g., vanillin), and bioactive compounds such as larvicides. This approach has evolved into a biorefinery framework, enabling the full valorization of biomass streams and the development of biomaterials, including bioplastics and biochars, applied in environmental remediation, energy, and agricultural systems.

More recently, biotechnological strategies involving cyanobacteria have expanded our capacity to generate sustainable bioproducts. These advances are supported by strong regional and national collaborations across Brazilian institutions, as well as international partnerships with Spain, Italy, Mexico, Thailand, Cameroon, Ecuador, Canada, France, and Australia—this latter contributing to high-impact scientific outputs. Such networks have significantly increased the depth, robustness, and global reach of our research.

By integrating local knowledge with global collaboration, this work reinforces the Amazon as a strategic frontier for sustainable technologies and bioeconomy-driven innovation.

Biography:

Associate Professor at the Federal University of Pará (UFPA), Brazil, and Deputy Director of the Institute of Biological Sciences (2025–2028). He holds a Ph.D. in Physical Chemistry at UFPA and completed postdoctoral research at the University of Córdoba, Spain. His research focuses on sustainable catalysis, biofuels, and biomass valorization, with emphasis on Amazonian resources. He is Vice-Coordinator of the Amazon Oils Laboratory, promoting collaboration between academia, industry, and local communities. He has held leadership roles in biotechnology programs at UFPA and serves as Guest Editor for international journals. He was awarded the Catalysis Researcher 2021 by the Brazilian Catalysis Society.

3DM Engineering: Accelerating Protein Engineering with AI for Next-Generation Biocatalysis

Tom van den Bergh*[1], Jeanine Boot[1], Bas Vroling[1], Bastiaan Brier[1], Henk-Jan Joosten[1]

[1]Bio-Prodict, Nijmegen, The Netherlands

Abstract:

Biocatalysis is playing an increasingly important role in enabling more sustainable chemical processes. However, engineering enzymes with the performance required for industrial application remains challenging, particularly when beneficial single mutations must be combined into higher-order variants with improved activity, selectivity, or stability. In practice, this often still depends on multiple rounds of library construction and extensive screening.

In this presentation, we will show how Bio-Prodict's 3DM Engineering platform provides a faster and more precise route to protein engineering. By combining protein family data integration, structure-based analysis, and artificial intelligence, 3DM Engineering identifies productive mutation combinations and designs improved enzyme variants without depending on large random libraries or lengthy iterative campaigns.

We will present how 3DM Engineering is used today to accelerate protein engineering and generate higher-order mutants with substantially improved performance. The platform reveals non-obvious combinations of mutations distributed across the protein structure, offering solutions that are difficult to derive using conventional rational design alone. Recent results show that 3DM Engineering can design five-mutation variants that outperform the best variants identified through conventional high-throughput screening. This illustrates how the approach can reduce screening effort, shorten development timelines, and increase the likelihood of identifying high-value variants for industrial biocatalysis.

This AI-driven workflow offers companies a scalable solution to accelerate enzyme optimization and advance biocatalyst development for sustainable chemistry applications.

Biography:

Dr. Tom van den Bergh is Head of 3DM at Bio-Prodict, where he leads teams working at the intersection of protein science, data integration, and AI-driven protein engineering. He focuses on translating protein family knowledge, structure-based analysis, and modern computational approaches into practical solutions for enzyme engineering and biocatalyst development. At Bio-Prodict, he is closely involved in the development and application of 3DM Engineering, a platform that combines data engineering, integration, and AI to accelerate protein optimization and support smarter design decisions in industrial biotechnology.

Supported Copper Catalysts for Sustainable C–H Amination and Selective Reductions Under Microwave and Flow Conditions

Katia Martina* Andrei Paraschiv, and Giancarlo Cravotto.

Department of Drug Science and Technology, University of Turin, Italy

Abstract:

Conventional synthetic protocols are increasingly being replaced by more efficient and sustainable approaches that employ safer reagents, readily available solvents, improved atom economy, and effective catalytic systems. In this context, copper and other 3d transition metals (e.g., Fe, Co, Ni, Mn) have emerged as valuable alternatives to noble metals (Pd, Pt, Rh), offering comparable catalytic performance alongside advantages such as natural abundance, low cost, and reduced toxicity.

In this work, two complementary applications of supported copper catalysts are presented: (i) C2 amination of benzoxazole and (ii) reduction of nitroarenes and alkynes to cis-alkenes. CuCl and $CuCl_2$ were efficiently immobilized on aminated silica and employed in microwave (MW)-assisted, additive-free amination of benzoxazole, affording excellent yields and broad applicability. In parallel, copper nanoparticles (CuNPs) supported on Celite were developed as efficient catalysts for hydride-free reduction of aromatic nitro compounds and semihydrogenation of alkynes.

Both methodologies demonstrated significant advantages in terms of safety, reaction rate, and product quality. The CuNP-based system was further adapted to continuous-flow conditions, where it showed high robustness and operational stability. The protocol is environmentally benign, avoiding the use of hydrogen gas and precious metals. Long-term studies confirmed sustained high conversions (>99%) over extended reaction times.

Finally, integration of microwave irradiation with flow processing (MW–Flow) led to a marked enhancement in productivity and catalytic efficiency, highlighting the potential of these systems for scalable and green chemical transformations.

Biography:

Dr. Katia Martina studied Chemistry and Pharmaceutical Technology at the University of Turin (Italy), where she obtained her Ph.D. in Chemistry. She then joined the Pharmacia & Upjohn Research Center in Nerviano (Milan) as a research scientist in the Chemistry Department. After seven years, she returned to the University of Turin, Department of Drug Science and Technology, where she was appointed Associate Professor of Organic Chemistry in 2020. Her research focuses on catalysis, functionalization of organic/inorganic materials, and innovative synthetic methodologies using non-conventional techniques, with particular expertise in microwave-assisted chemistry, sonochemistry, and flow chemistry.

A Zinc-Based Catalyst for the Synthesis and Chemical Recycling of Polyester

Federica Santulli*, Marina Lamberti, Mina Mazzeo

Department of Chemistry and Biology "Adolfo Zambelli", University of Salerno, Italy

Abstract:

Aliphatic polyesters have emerged as a highly promising class of bioplastics due to their renewable origin and inherent biodegradability. However, their end-of-life management remains a significant challenge: under natural conditions, degradation is often slow, while industrial composting processes can be energy-intensive and inefficient. For this reason, catalytic systems that can bridge polymer synthesis and chemical recycling are particularly appealing.[1]

In this work, we present a zinc complex bearing phenoxy-imine-pyridine ligand that efficiently catalyzes the ring-opening polymerization of cyclic esters under conditions relevant to industrial practice, offering a less toxic alternative to traditional tin-based catalysts. Remarkably, the same catalyst can also be used for the chemical recycling of aliphatic polyesters *via* hydrolysis and alcoholysis, producing the corresponding hydroxycarboxylic acids and alkyl esters, respectively, under mild conditions.[2] In addition, under reduced pressure, it enables direct depolymerization back to the original cyclic monomers, supporting a closed-loop recycling approach.

Biography:

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[2] Santulli, F.; Gravina, G.; Lamberti, M.; Tedesco, C.; Mazzeo, M. Mol. Catal. 2022, 528, 112480.

Chitosan from Insects: Versatile Role in Green Chemistry and Circular Economy

Ana P.C.Ribeiro* Luísa M.D.R.S. Martins[1,2] and Andreia O. Figueiras[1]

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[2] *Department of Chemical Engineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1, Lisboa 1049-001, Portugal*

Abstract:

Chitosan derived from insects has gained increasing attention as a sustainable biomaterial supporting green chemistry, circular economy strategies, and catalytic applications. Traditionally sourced from crustacean waste, chitosan can be efficiently extracted from insect biomass such as black soldier flies and mealworms, offering a renewable alternative that reduces pressure on marine ecosystems. This approach aligns with circular economy principles by valorizing organic waste streams used in insect farming and converting them

into high-value products. Insect-derived chitosan retains key properties including biodegradability, biocompatibility, and functional versatility, enabling its use across environmental, agricultural, and biomedical fields. Notably, its chemical structure, rich in amino and hydroxyl groups, makes it an excellent support or active component in catalysis. Chitosan-based catalysts have been applied in heterogeneous catalysis, metal ion immobilization, and green synthesis reactions, enhancing efficiency while minimizing toxic byproducts. Additionally, its role in water treatment as both an adsorbent and catalytic material further highlights its multifunctionality. The integration of insect-derived chitosan into industrial processes promotes waste reduction, resource efficiency, and the substitution of non-renewable materials. Overall, it represents a promising pathway toward sustainable production systems, bridging biotechnology, environmental protection, and green catalytic innovation in a circular economy framework.

Biography:

Ana Paula Ribeiro holds a degree in Chemistry and a Master's in Materials from the Faculty of Sciences, University of Lisbon, a European Master in Computational Simulation and Theoretical Chemistry from the University of Perugia, and a PhD in Chemistry from FCUL. She is an Auxiliary Researcher at Centro de Química Estrutural and Invited Assistant Professor at Instituto Superior Técnico. Her research focuses on green chemistry, ionic liquids, and sustainable catalysis, including mechanochemistry and sonochemistry. She has authored 105 papers, holds 4 patents, contributed 12 book chapters, and delivered over 190 conference presentations.

Cascade Biorefining of Wet Agro-Industrial Residues into Renewable Energy Carriers: Integrated Extraction, Ni-Catalyzed Supercritical Water Gasification and Mn–Ce Catalyzed Wet Air Oxidation

Catia Cannilla*, Mario Samperi, Serena Todaro, Mariarita Santoro, Chiara Corrente, Francesco Arena, Alessandro Cajumi, Giuseppe Bonura

Institute of Advanced Technology for Energy CNR-ITAE "Nicola Giordano", Messina, Italy

Abstract:

The efficient valorisation of wet agro-industrial residues is a critical challenge due to their high water content, low energy density and complex composition. Here, a cascade biorefinery approach is proposed, integrating extraction, supercritical water gasification (SCWG) and catalytic wet air oxidation (CWAO) for the simultaneous recovery of value-added compounds and production of renewable energy carriers. Citrus processing residues (pastazzo) and spent

brewery grains were selected as representative feedstocks. A preliminary extraction step, performed using green solvents and intensified techniques, enables the recovery of high-value biomolecules while preserving most of the organic carbon for downstream conversion. The extracted residues are subsequently processed via SCWG using Ni-based catalysts supported on different oxides and prepared through tailored synthesis routes. The use of non-noble metal catalysts, combined with structured configurations, allows improved control of product distribution toward H_2- or CH_4-rich gas streams under severe conditions, while enhancing catalyst stability in the presence of inorganic contaminants. The aqueous phase produced after SCWG is further treated by catalytic wet air oxidation using Mn–Ce based catalysts, enabling the efficient removal of refractory organic compounds and supporting water reuse within the process. Advanced physico-chemical characterization, including in situ and operando spectroscopy combined with advanced electron microscopy, was employed to establish structure–activity relationships and elucidate the role of metal–support interactions in governing catalytic performance. Overall, the proposed cascade biorefinery demonstrates a robust and integrated strategy for the near-zero-waste valorisation of wet agro-industrial residues, combining chemical recovery, renewable energy carriers production and wastewater treatment within a circular economy framework.

This research was funded by the programme Ricerca di Sistema PTR25-27 and Fondo Italiano per la Ricerca through the project SUPERBIO (FIS00002427).

Biography:

Dr. Catia Cannilla is a Senior Researcher at CNR-ITAE. She obtained her PhD in Chemical Technologies and Innovative Processes at the University of Messina. Her research focuses on heterogeneous catalysis for energy applications, particularly on the design of advanced catalytic materials for the production of clean fuels. She has developed strong expertise in advanced bulk and surface physico-chemical characterization techniques, including in situ and operando methodologies. She is Scientific Responsible of various research projects, being actively involved in several national and international collaborations with academic and research institutions.

Catalytic Upcycling of Plastic Waste *via* Biochar-Enhanced Microwave-Assisted Co-Pyrolysis

Matteo Francavilla1*, Tayyaba Gull1, Paolo Marasco1, Mauro Marone1, Mario Fedele2, Marcello Salvatori2

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Abstract:

Plastic waste accumulation represents a major environmental challenge, while current recycling rates remain insufficient to mitigate its long-term ecological impact. In this work, microwave-assisted co-pyrolysis (MAP) is proposed as a sustainable route for the upcycling of plastic waste into energy carriers and carbonaceous products, using residual biomass-derived biochar as both microwave susceptor and low-cost catalytic material. Biochars were produced from different feedstocks, including olive prunings, wood prunings, blue crab shells, and the red seaweed Gracilaria gracilis, and subsequently assessed in terms of physicochemical properties, structural features, and microwave absorption behaviour.

MAP experiments were carried out in a Pyrowave microwave muffle using plastic samples, mainly high-density polyethylene, blended with biochar at a 7:3 weight ratio. The mixtures were processed at temperatures between 400 and 800 °C under different residence times to evaluate the influence of operating conditions on product distribution. Increasing temperature promoted gas formation, whereas lower temperatures favoured the production of solid residues. Particular attention was devoted to hydrogen and methane generation, with optimized conditions yielding an H_2/CH_4 molar ratio up to 2.08 at 550 °C after 1 h of residence time.

FTIR analysis of plastics and biochars supported the interpretation of the main chemical transformations occurring during co-pyrolysis. The results demonstrate that biochar can

efficiently enhance microwave heating and influence cracking and reforming pathways, improving the conversion of plastic waste into valuable products. Overall, this study highlights the potential of biochar-assisted MAP as a circular and energy-efficient strategy for plastic waste valorisation, clean fuel production, and sustainable waste management.

Biography:

Matteo Francavilla is Associate Professor of Organic Chemistry at the Department of Agricultural Sciences, Food, Natural Resources and Engineering (DAFNE), University of Foggia. He is Scientific Coordinator of the STAR*Facility Centre, a national research infrastructure (PNIR 2021/27 - MUR) focused on biomass and by-product valorisation through biorefinery processes, and Vice President of AISAM. His research focuses on green chemistry, blue biotechnology and circular bioeconomy, with particular attention to the sustainable conversion of agro-industrial biomass, macroalgae and microalgae into high-value compounds and bio-based products. He has coordinated and contributed to several national and international research projects.

Oral Talks

High-Entropy Oxides as Electrocatalysts in Anion Exchange Membrane Water Electrolyzers for Green Hydrogen Production

Maria Grazia Musolino[1]*, Sabrina Campagna Zignani[2], Marta Fazio[2], Mariarosaria Pascale[2], Chiara Alessandrello[1], Claudia Triolo[1] and Saveria Santangelo[1]

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Abstract:

Anion exchange membrane water electrolysis (AEMWE) stands out as a promising low temperature technology for cost-effective and sustainable hydrogen production, due to its ability to use non-precious metal catalysts, working in alkaline environment, and to produce high purity hydrogen. Nevertheless, its practical application still encounters considerable kinetic challenges, relying on electrochemical energy to drive the cathodic hydrogen evolution reaction (HER) and the anodic oxygen evolution reaction (OER), so leading to poor electrolysis efficiency. Then, the rational design and development of highly active, durable and eco-friendly electrocatalysts is a crucial challenge to advancing of this technology. Recently, the emergence of multi-metallic nanomaterials based on the high-entropy concept has opened a new paradigm for catalyst design. Unlike conventional low- or medium-entropy oxides, high-entropy oxides, consisting of five or more principal elements in equimolar or near-equimolar ratio, dissolved in a single lattice, are endowed with excellent thermodynamic stability and enhanced catalytic performance. This study focus on the synthesis and characterization of nanostructured (Cr,Mn,Fe,Co,Ni)-based high-entropy oxides and their testing as electrocatalysts in a zero gap AEMWE electrolyzer. High-entropy oxides are synthesized via a sol-gel technique, followed by calcination at different temperatures (400, 500, 600 or 800 °C). The as-prepared oxide is utilized to fabricate the anode of a zero-gap AEMWE full cell, while for the fabrication of the cathode the oxide is first reduced in a H_2/Ar atmosphere. The effect of calcination temperature on the electrochemical cell performance, as resulting from the physicochemical properties of the obtained electrode materials, is investigated.

Biography:

Maria Grazia Musolino is currently Associate Professor of Chemical Fundamentals of Technologies at the Mediterranean University of Reggio Calabria since 2007. Her research focuses mainly on sustainability issues, in particular the synthesis and characterization of (nano)materials for catalytic and energy-related applications. She is author of about 50 publications in peer-reviewed international scientific journals, 2 book chapters, and about 115

communications at scientific conferences. She is Guest Editor of 3 Special Issue in Nanomaterials, MDPI.

Transformation of α-Pinene to High Value-Added Molecules on Carbon-Supported Noble Metals

Filippo Ravasio1*, Katharina Konieczny1, Tianyin Qiu2, Janpaul Menzel2, Victor S. Batista2, Eszter Baráth1

1Leibniz-Institut für Katalyse e.V. (LIKAT), Germany; 2Yale University, USA

Abstract:

Turpentine, a waste product from the forest industry that is underutilized, contains high amounts of α-pinene which can be used to obtain high-value products. *Cis*-pinane, for example, is a valuable intermediate widely used in chemical and pharmaceutical synthesis which can be obtained through the selective hydrogenation of α-pinene. Here, we propose a systematic study on the selective conversion of α-pinene to *cis*-pinane, examining both direct hydrogenation conditions (1 bar of H_2 gas) and catalytic transfer hydrogenation (CTH) using various alcohols as hydrogen donors, with Pt/C and Ru/C catalysts. The hydrogen donors tested were primary and secondary alcohols. Regardless of the chain length or metal used, primary alcohols were entirely inactive in CTH. Conversely, secondary alcohols exhibited complete conversion with Ru/C. Overall, CTH and direct hydrogenation with Ru/C exhibited higher selectivity towards the *cis* isomer compared to Pt/C. The activation parameters of the reaction were determined to rationalize this behavior. Based on the activation parameters of Ru/C the use of H2 gas does not exclude the possibility of CTH occurring during the reaction. For this reason, isotope labeling experiments were carried out to gain deeper mechanistic insights. Using D2 as a hydrogen source we observed a small amount of deuterated products in the case of Ru/C, confirming that CTH is as fast as direct hydrogenation. Finally, the binding energies of the different hydrogen donors for the two catalytic systems were calculated using DFT to elucidate the observed differences in selectivity and activity between the two metals.

Biography:

Filippo Ravasio is a second year PhD candidate in the Department of Synergies in Catalysis at Leibniz-Institut für Katalyse e.V. (LIKAT), working under the supervision of Prof. Dr. Eszter Baráth. The research focuses on transfer hydrogenation with heterogenous catalyst on biomass derived substrate. Prior to their doctoral studies, Filippo Ravasio received a MSc in Chemistry from Università degli Studi di Milano.

Computational Insights into the Catalytic Reduction of Furfural Over Co-Based Oxides

Pierraffaele Barretta*[1], Giulia Maria Itri[2,3], Tapio Salmi[4], Andrea Donato[2], Adriana Pietropaolo[1], Chiara Alessandrello[2], Claudia Triolo[2], Francesco Mauriello[2] and Emila Paone[2].

[1]Dipartimento di Scienze della Salute, Università Magna Graecia di Catanzaro, Italy;
[2]Dipartimento DICEAM, Università degli studi Mediterranea di Reggio Calabria, Italy;
[3]Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, Italy;
[4]Laboratory of Industrial Chemistry and Reaction Engineering (TKR) Åbo Akademi University, Finland.

Abstract:

Biomass-derived furfural is a key platform molecule for the sustainable production of furfuryl alcohol, a critical intermediate for biofuels and green chemicals. While noble metal catalysts dominate this transformation, earth-abundant cobalt-based oxides have emerged as promising alternatives, exhibiting strong structure-activity relationships that govern selectivity between carbonyl hydrogenation and deeper deoxygenation pathways. Oxygen vacancies and redox-active surfaces have been identified as critical descriptors for H_2 activation, yet their precise mechanistic role at the atomic scale remains poorly understood. Here, we present a comprehensive computational investigation of furfural hydrogenation over two different phases of $LiCoO_2$, the layered $R\bar{3}m$ and the spinel-like $Fd\bar{3}m$ benchmarked against Co_3O_4, and CoO. Using density functional theory combined with machine learning interatomic potentials and well-tempered metadynamics, we map the full free-energy landscapes of competing reaction pathways and identify the key descriptors governing catalytic activity and selectivity. Our results reveal that $Fd\bar{3}m$ $LiCoO_2$ dramatically lower the activation barriers for H_2 dissociation and carbonyl hydrogenation, with the lowest adsorption energy, outperforming conventional cobalt oxides in both activity and selectivity toward furfuryl alcohol. These findings are rationalized through a unified structure-activity framework and validated against experimental data. This work establishes $Fd\bar{3}m$ $LiCoO_2$ as a high-performance, waste-derived catalyst for biomass valorization, offering a compelling proof of concept for integrating battery recycling into circular and sustainable chemical processes.

Techno-Economic Considerations for Production of Commodities/Specialty Chemicals Using Immobilized Biocatalysts [Online]

Ronaldo Pio Rodrigues de Sousa*

National National Institute of Technology (INT), Brazil

Stereoselective Bio-Organocatalytic Cascade to Chiral Amides as API Intermediates Using ω-Transaminase and Choline Chloride Under Microwave Irradiation

Salvatore Romano,[a,b,*] Matteo Damian,[a,‡] Monica Nardi,[b] Antonio Procopio,[b] Sebastian Strähler,[c,d] Daniël Preschel,[c] Manuela Oliverio*[b] and Francesco G. Mutti *[a]

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[d] S. Strähler, Institute of Condensed Matter and Nanosciences, Molecular Chemistry, Materials and Catalysis (IMCN/MOST) Université Catholique de Louvain 1348, Louvain-la-Neuve, Belgium

Abstract:

Amide bond formation remains a cornerstone transformation in pharmaceutical synthesis, yet conventional methods rely heavily on stoichiometric activating reagents, hazardous solvents, and energy-intensive conditions. Here we report a fully integrated bio-organocatalytic cascade that couples stereoselective ω-transaminase (ω-TA) transamination in neat organic solvent with choline chloride (ChCl)–mediated direct amidation under solvent-free microwave irradiation. This approach enables the efficient synthesis of highly enantioenriched chiral amides directly from simple prochiral carbonyl compounds and carboxylic acids, providing a streamlined and sustainable alternative to traditional amide-forming methodologies. Biocatalytic optimization in MTBE allowed both Cv-ωTA and AsR-ωTA to operate with excellent conversions (>99%) and enantiomeric excess (97–>99% ee), even with sterically demanding substrates. We identified MTBE as the optimal medium, balancing enzyme flexibility, substrate solubility, and operational practicality. Subsequent solvent evaporation proved essential to remove acetone generated from the amine donor 2-propylamine and to enable efficient ChCl coordination in the organocatalytic step. Under microwave irradiation (80 °C, 18 min), the amidation proceeded smoothly across a broad range of aliphatic and aromatic carboxylic acids, delivering the target amides in 60–86% isolated yields. The cascade was successfully applied to the synthesis of key chiral building blocks of racecadotril and AVR-48, demonstrating its relevance to API intermediate preparation. Notably, both enantiomers of the amine intermediates were processed without

loss of stereochemical integrity, highlighting the robustness of the method. Overall, The combination of ω-TA catalysis, ChCl-mediated activation, and microwave irradiation represents a promising platform for sustainable pharmaceutical manufacturing and future process intensification.

Biography:

I obtained my PhD from University Magna Graecia of Catanzaro in life sciences in 2024. I did a postdoc at the Green Laboratory of the University Magna Graecia of Catanzaro until august 2025, focused on the developing of Eco-sustainable technologies for separating, recovering, and transform lignin from biomass. Starting from October 2025 I joint the Biocatalysis group because I've won a post-doctoral fellowship grant as part of the EU Marie Skłodowska-Curie. In my research will integrate biocatalysis and organocatalysis, starting by combining the use ofdifferent type of enzymes for production of important molecules with a green method using choline chloride-DES.

Advanced MnOx-Based Catalysts for PROX: Bridging Theory and Application

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Abstract:

Hydrogen is widely regarded as a key energy carrier in the transition toward more sustainable energy systems. However, hydrogen produced by conventional hydrocarbon reforming processes typically contains residual carbon monoxide (CO), which prevents its direct use in proton exchange membrane fuel cells (PEMFCs) due to Pt electrode poisoning. Among the available purification strategies, the preferential oxidation of CO (PROX) has emerged as a promising solution, although the development of efficient, selective and low-cost catalysts remains a major challenge. In this work, a nanocomposite MnCeOx catalyst was investigated through a combined experimental and computational approach to assess its potential for PROX applications. The catalyst, synthesized by redox-precipitation, was extensively characterized, highlighting the key role of surface Mn(IV) species in determining its catalytic behavior. Catalytic tests revealed high CO oxidation activity at low temperature (293 K) together with negligible hydrogen oxidation below 373 K, resulting in a favorable PROX response in the 293-423 K range. To rationalize these results, Density Functional Theory (DFT) calculations were performed on a Mn4O8 cluster model. The calculations showed that Mn(IV) sites interact with CO and H2 through distinct pathways, giving rise to two separate oxidation cycles with significantly different activation barriers. This energy gap explains the observed

selectivity toward CO oxidation. Experimental and theoretical results were further integrated into simplified reaction mechanisms and kinetic models capable of describing both CO and H2 oxidation in the 293-533 K range. Overall, this study provides mechanistic insight into MnCeOx catalysts and offers a rational framework for designing selective mixed-oxide catalysts for hydrogen purification.

This research was funded by the programme Ricerca di Sistema PTR25-27.

Biography:

Dr. Alessandro Cajumi is a chemist, with a specific background in nanotechnology and supramolecular chemistry. In 2026 he received his PhD in Industrial and Information Engineering at the University of Messina. Currently, he is a research scientist at CNR-ITAE, Messina, involved in the synthesis, characterization and testing of solid catalytic systems for the conversion and valorization of by-products and waste biomass into clean alternative fuels.

Partial Hydrogenation of Alkynes Using Carbohydrates as Alternative Hydrogen Source on Pt/C

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Abstract:

The selective semi-hydrogenation of alkynes is one of the most important organic transformations with wide applications.1 The direct application of biomass in transfer hydrogenation reactions is beneficial because of renewability. Biomass derived hydrocarbons, such as sugars, cellulose, and starch, are potentially important feedstocks obtained by photosynthesis in plants from CO2. For instance, glucose is inexpensive, easily obtained from natural renewable resources, and safe to handle. This method has the advantage of eliminating the use of pressurized H2 gas and related pressure-accommodating experimental setups.2

The transfer hydrogenation of alkynes with carbohydrates exhibited a highly selective saturation pattern, where the cis-alkene was the predominant intermediate and the trans-alkene a minor product (Figure 1). The formation of the corresponding fully saturated product was not observed.

We analyzed the carbohydrate after the reaction. In a model reaction, we detected small, oxidized fragments like lactic acid, still intact six membered sugar molecules and oxidized six membered sugar rings.

We tested various carbohydrates for the transfer hydrogenation of internal alkynes in a wide substrate scope. In order to determine the physical chemical parameters of the given reaction, diphenylacetylene, as model compound was studied. Kinetic analysis revealed initial reaction rates and activation parameters, including activation energy (Ea), activation enthalpy (ΔH‡), and activation entropy (ΔS‡).

Monosaccharides, disaccharides and polysaccharides were used successfully as H-donors in this model reaction. Under optimized conditions 35 differently substituted internal alkynes were studied, the corresponding cis/trans alkenes were detected with good to excellent yields.

In order to utilize the sugar residue remaining after the reaction, we followed a protocol for the synthesis of bio-derived carbon with a high surface area, which can be used as a supporting material in catalyst synthesis.

1 Kusy R.; Grela, K. Chem. Rev. 2025, 125 (9), 4397-4527

2 Manna S.; Antonchick A. P. ChemSusChem 2019, 13, 3094-3098

Catalytic Pyrolysis of Mixed Plastic Waste in a Two-Stage Fluidized Bed Reactor

Piotr Trochimczyk[1,2]* and Krzysztof Krawczyk[1]

[1]Warsaw University of Technology, Faculty of Chemistry and [2]MARTEX

Abstract:

Global plastic production reached 413.8 million tons in 2023, and only 9% of plastics are recycled. The complexity of municipal waste streams limits the effectiveness of mechanical recycling. Our research focuses on chemical recycling as a solution to the surge in mixed plastic waste. We have designed and tested a two-stage fluidized bed reactor for the catalytic pyrolysis of a mixed plastic simulating municipal collection (PE, PP, PET, and PS).

The central innovation of this work is the implementation of a two-stage catalytic system that uses a custom-synthesized Ni/γAl_2O_3 catalyst in the first stage and an industrial G-0110 nickel catalyst in the second stage. Our process operates at atmospheric pressure with temperatures ranging from 400°C to 453°C, which is significantly lower than the usual 800°C required for non-catalytic thermal pyrolysis. Nickel was selected for its established utility in the petrochemical sector and its cost-effectiveness.

Reactor demonstrated high efficiency in cracking plastic into hydrocarbons, yielding 90.33 +/- 1.41 of oil and waxes. Syngas or combustible gases at 2.00 +/- 0.92 yield, and char carbonaceous residues yielding 7.67 +/- 0.53. GC-MS confirmed that the liquid and wax

fractions contain a rich mixture of aliphatic and aromatic hydrocarbons, including styrene, toluene, indene, and benzoic acid. Our study provides empirical evidence that a two-stage catalytic system can overcome the challenges of mixed plastic pyrolysis. As the petrochemical industry moves toward mandatory recycled-content requirements, our fluidized bed technology offers a scalable, efficient pathway to transform global waste liability into a valuable industrial asset.

Biography:

I am a scientist and entrepreneur dedicated to bridging the gap between academic research and industrial application. I am a doctoral researcher at the WUT, specializing in Chemical Technology. My scientific focus lies in catalysts, polymers, and the pyrolysis of plastic waste. I used to work for the IPC PAS, where I ran or participated in 3 grants. I have authored seven scientific publications in international journals.

I serve as an executive at MARTEX. By integrating my technical expertise into business ventures, I aim to drive innovation in the plastics industry, turning advanced chemical research into practical solutions.

Fatty Acid Upgrading to Linear Olefins Over Aminophosphine-Derived Precatalysts

Sibongile Pikoli[1,2*] and Banothile CE Makhubela[1]

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Abstract:

Fatty acid dehydrative-decarbonylation presents a sustainable route for producing value-added linear alpha-olefins. Alkenes form the fundamental building blocks for organic synthesis and industrial applications from fuels, fine chemicals and pharmaceuticals. Traditionally, long-chain olefins are produced form the oligomerization of ethylene which is sourced from fossil fuel. Herewith we report the synthesis, characterization and application of phosphino-amine complexes, PdL, IrL, and CoL, as precatalysts in the dehydrative-decarbonylation of C_{18} fatty acids. This method reduces the excess phosphine addition typical for in situ generated catalysts in this process that lead to higher production costs, waste and inhibit industrial adoption. The reaction pathway and product selectivity are demonstrated to be influenced by the metal center and coordination environment. The Ir^{3+} complex exhibited the highest activity (95.9 % conversion) and linear α-olefins selectively (62.7 %), while Pd and Co complexes primarily yielded aldehydes at 67.3% and 64.5, respectively. We propose the aldehyde production pathway takes place via the reaction of alkyl radical intermediates and side-products. Immobilization of the Pd complex onto SBA-15 resulted in a tandem alkene and ketone generation, demonstrating the tunable selectively of these catalysts. HR-TEM analysis

of the recovered heterogeneous catalyst depicted nanoparticle formation, recognized to favor decarboxylation over decarbonylation. This work illustrates the capacity of phosphinoamine-derived complexes as adaptable catalysts in the sustainable deoxygenation of fatty carboxylic acids.

Biography:

Sibongile Pikoli, born in Gqeberha, South Africa, earned her PhD in Chemistry from the University of Johannesburg in 2025. After which she joined the University of South Africa as a postdoctoral fellow at the Institute of Catalysis and Energy Solutions (ICES). Her research specializes in catalysis and process optimization, with a strong focus on designing efficient and sustainable chemical processes. She has published peer-reviewed work on catalyst development and the reaction mechanisms involved in lipid deoxygenation and has shared her findings at several international sustainability forums. Passionate about green chemistry and catalysis, Sibongile is dedicated to bridging the gap between laboratory research and industrial application.

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