

2nd International Conference on **Catalysis Science and Chemical Engineering**

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Abstract book



Day 1

Plenary Session

Electrocatalytic Refinery for Production of Fuels and Chemicals

Shi Zhang Qiao*

The University of Adelaide, Australia

Abstract

Compared to modern fossil fuel-based industrial refineries, the emerging electrocatalytic refinery (e-refinery) is a more sustainable and environmentally benign strategy to convert renewable feedstocks and energy sources to transportable fuels and value-added chemicals. E-refinery promisingly leads to defossilization, decarbonization, and decentralization of chemical industry. Specifically, powered by renewable electricity (e.g., solar, wind and hydro power), oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) can efficiently split water into green hydrogen and CO₂ reduction reaction (CRR) can convert CO₂ emissions to transportable fuels and commodity chemicals.

A crucial step in realizing this prospect is the knowledge-guided design of appropriate reactions and optimal electrocatalysts with high activity and selectivity for anticipated reaction pathways, which dominantly involve cleavage and formation of chemical bonds between H, O and C. In this presentation, I will talk about our recent progress in mechanism understanding and material innovation for some crucial electrocatalytic reactions (OER, HER, CRR, etc.), which are achieved by combining atomic-level material engineering, electrochemical evaluation, theoretical computations, and advanced *in situ* characterizations. A special emphasis is placed on the rational exploration of novel single-atom catalysts.

Biography:

Dr. Shizhang Qiao is a Chair Professor at the School of Chemical Engineering, the founding Director of the Center for Materials in Energy and Catalysis (CMEC), and Director of ARC Industrial Transformation Training Centre for Battery Recycling, at the University of Adelaide (UoA), Australia. His research expertise lies in nanostructured materials for electrocatalysis, photocatalysis, batteries, and other new energy technologies. He has co-authored 550 papers in refereed journals with 135,000 citation times, resulting in an h-index of 185.

Hydrogen Generation by Water Electrolysis

Zhifeng Ren*

University of Houston, USA

Abstract

Hydrogen (H₂) has a very high energy density and is environmentally friendly when it is used as fuel because the byproduct is the purest water, but the current way to commercially produce H₂ using fossil fuels via. gas reforming and coal gasification is not sustainable due to the production of a vast amount of CO₂. On the other hand, water electrolysis using the over supplied grid power during the offpeak hours and renewable energy from solar and wind is not only clean but also economical if high performance catalysts for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) can be made in large scale at a low price. In this talk I will present our effort on studying water treatment, efficient catalysts, and electrolyzer designing for water electrolysis, especially seawater due to the abundance supply than the fresh water.

Biography:

Zhifeng Ren is the Paul C. W. Chu and May P. Chern Endowed Chair in Condensed Matter Physics in the Department of Physics and the Director of the Texas Center for Superconductivity at the University of Houston (TcSUH). He received his BS in 1984 from Xihua University, MS in 1987 from Huazhong University of Science and Technology, and PhD in 1990 from the Institute of Physics, Chinese Academy of Sciences. His research focuses on catalysis for water electrolysis, thermoelectrics with high ZT and power factor, boron arsenide single crystals for high thermal conductivity and carrier mobility, enhanced oil recovery, heated HEPA filters for catching and killing SARS-CoV-2 causing COVID-19 pandemic, carbon nanotubes, solar absorbers, flexible transparent conductors, superconductors, *etc.*

Strain Catalysis for Hydrogen Cycles

Shaojun GUO*

Peking University, China

Shaojun GUO is a Boya Distinguished Professor in Peking University, and a Fellow of the Royal Society of Chemistry. He is renowned for his outstanding contribution to the interdisciplinary fields of materials chemistry for energy electrocatalysis. He has published more than 200 papers in top journals as corresponding author, including 40 in Nature, Science and Nature/Science/Cell sister journals (h-index=144 and 74,000 citations). He is one of Highly Cited Researchers from 2014 to 2023, and World Top 2% Scientist from Stanford University (Ranking: 2000). His selected awards/honors include Xplorer Prize, National Science Fund for Distinguished Young Scholars, China Youth Science and Technology Prize, Elsevier Chinese Most Cited Researcher, etc. He is serving as (advisory) board members of Adv. Energy Mater., Chem. Commun., Sci. Bull., Sci. China Mater., eScience, etc

Emerging Energy Electrocatalysis for Rechargeable Batteries

Chang Xin Zhao, Bo Quan Li, Jia Ning Liu, and Qiang Zhang*

Tsinghua University, China

Abstract:

Sustainable energy supply and sufficient chemical production are highly dependent on many essential catalytic processes for our sustainable society. For instance, lithium–sulfur (Li–S) batteries constitute promising next-generation energy storage devices due to the ultrahigh theoretical energy density of 2600 Wh kg⁻¹. However, the multiphase sulfur redox reactions with sophisticated homogeneous and heterogeneous electrochemical processes are sluggish in kinetics, thus requiring targeted and high-efficient electrocatalysts. A family of energy electrocatalyst is designed to tailor the characters of the sulfur redox reactions in working Li–S batteries. The efficiency of the electrocatalysis regulated by Li bond interactions is further verified in practical Li–S batteries that realize superior rate performances and long lifespan as well as high-energy-density Li–S pouch cell. This talk not only proposes an efficient electrocatalyst design strategy to promote the Li–S battery performances but also inspires electrocatalyst development facing analogous multiphase electrochemical energy processes.

Biography:

Prof. Qiang Zhang is a full professor at Tsinghua University. He obtained his Ph.D. in chemical engineering (2009) from Tsinghua University, China, and subsequently held Research Associate/Postdoc Research Fellow positions in the Case Western Reserve University, USA, and Fritz Haber Institute of the Max Planck Society, Germany. He held the Newton Advanced Fellowship from Royal Society, UK and the National Science Fund for Distinguished Young Scholars. He is selected as highly cited researchers at 2017-2023 by Clarivate Analytics. His current research interests are advanced energy materials, including dendrite-free lithium metal anode, lithium sulfur batteries, and electrocatalysis, especially the structure design and full demonstration of advanced energy materials in working devices. His h-index is 169 now. He is the Advisor Editor of *Angew. Chem.*, Associate Editor of *J Energy Chem*, *EcoMat*, & *Energy Storage Mater*. He is sitting on the advisory board of *Chem Soc Rev*, *Joule*, *Matter*, *Adv Funct Mater*, *ChemSusChem*, *J Mater Chem A*, *Chem Commun*, and so on. He is the deputy head of the expert group on energy storage and smart grid of the national key research and development plan. He has won the first prize of Natural Science of the Ministry of Education, the first prize of Fundamental Science of the Chemical Engineering Society.

Functional Carbon Materials for Catalysis

Jieshan Qiu*

Beijing University of Chemical Technology, China

Abstract

Functional carbon materials with tuned structure and properties are of great potential in many fields, which can be produced from different carbon-containing precursors by various technologies. By making use of molecular chemical engineering methods including molecular science, surface and interface engineering, multi-dimension carbon materials with engineered functionalities have been fabricated and demonstrated to enable advanced catalysis for production of fine chemicals and for electro-conversion of CO₂ and N₂ molecules.

Biography:

Jieshan Qiu, Cheung-Kong Distinguished Professor of Carbon Science and Chemical Engineering at Beijing University of Chemical Technology, China. His research encompasses both fundamental and applied aspects of carbon materials and science, with a focus on the methodologies of producing carbon materials for energy storage and conversion, catalysis, and environment protection. He has published 900⁺ papers in peer-reviewed journals, including *Nature Mater.*, *Adv. Mater.*, *Adv. Funct. Mater.*, *Adv. Energy Mater.*, *Energy Environ. Sci.*, *PNAS*, *Nature Commun.*, *ACS Nano*, *Angew. Chem. Int. Ed.*, *J. Am. Chem. Soc.*, *Joule*, *Matter*, *Chem*, etc., with citations 67000⁺ times and h-index of 127 (google scholar), and his work has been featured on 70 covers of international journals. He has been invited to give 160⁺ plenary/invited/keynote talks in conferences and at universities and research institutes. He has filed 170⁺ Chinese and International patents. He has been honored with 30⁺ prestigious awards and prizes including the First-class award for fundamental research and industrialization technologies from the Education Ministry of China and Liaoning Province. He is a highly cited researcher by Clarivate Analytics from 2018 to 2023 and by Elsevier from 2019 to 2023. Right now, he is the Associate Editor of *Battery Energy* (Wiley) and *Chemical Engineering Science* (Elsevier).

Visible Light-Induced Asymmetric Radical Reactions Catalyzed by Chiral *N,N'*-Dioxide-Metal Complexes

Xiaoming Feng*

Sichuan University, Chengdu, China

Abstract

Visible light photocatalysis holds a prominent position in modern synthetic chemistry, offering exciting opportunities to build new catalytic platforms, which is complementary or sometimes even superior to thermocatalysis. Nevertheless, the stereocontrol in visible light photoinduced asymmetric radical reactions remains a formidable challenge, mainly due to the highly reactive and short-lived radical species, leading to nonnegligible side reactions and the uncontrolled racemic background reaction as well as the low reaction barriers for difficulty in fine discrimination of face selectivity. In the past two decades, our group has developed a novel type of conformationally flexible chiral *N,N'*-dioxide-amide compounds, which are recognized as newly privileged chiral ligands and referred as “Feng ligand” and can coordinate with metal ions to form effective chiral Lewis acid complexes, enabling 70 types of asymmetric reactions. Recently, the chiral Feng *N,N'*-dioxide/metal complex catalysts were employed in visible light photocatalysis to mediate the previously unattainable organic transformations in the ground-state domain, including alkylation of ketones and imines, radical addition to α,β -unsaturated carbonyl compounds as well as cycloaddition of indole derivatives and simple alkenes.

Biography:

Xiaoming Feng received his B.S. (1985) and M.S. degrees (1988) from Lanzhou University. In 1996, he received his Ph.D. degree from the Institute of Chemistry, CAS. He worked at the Chengdu Institute of Organic Chemistry, CAS (1996–2000) and was appointed as a professor in 1997. He did postdoctoral research at Colorado State University (1998–1999). In 2000, he joined Sichuan University as a professor. In 2013, he was selected as a member of Chinese Academy of Sciences. His research interests include the design of chiral catalysts, development of new synthetic methods and synthesis of bioactive compounds.

Session: Green Synthesis, Catalysis and Electrochemical Reactions

Keynote Talk

Green Methods in the Synthesis of Organophosphorus Compounds with potential Bioactivity

Gyorgy Keglevich*

Budapest University of Technology and Economics, Hungary

Abstract:

The microwave (MW) technique has become an important tool in organophosphorus chemistry. In this lecture, the advantages of MWs in different reactions are surveyed allowing green chemical accomplishments. The first case is the MW-assisted direct esterification of phosphinic¹ and phosphonic acids,² along with phosphoric ester-acids³ that all became more efficient in the presence of an ionic liquid catalyst. The O-alkylation of phosphonic acids and phosphoric ester-acid derivatives under MW irradiation is also a useful technique.⁴ The interconversion of phosphinates and phosphinic amides was also elaborated.⁵ Alcoholyses and hydrolyses of P-esters were also investigated and optimized.^{6–8} A valuable finding of ours is that in the Hirao P–C coupling of >P(O)H reagents and bromoarenes applying Pd(OAc)₂ as the catalyst, the slight excess of the >P(O)H species may substitute the usual P-ligands in the tautomeric >POH form.⁹ Ni-catalyzed cases will also be shown. The latter variation involves a brand new mechanism assuming a Ni(II) → Ni(IV) transition.¹⁰ Heterocyclic derivatives were also involved in P–C couplings to provide P-functionalized species with cytostatic activity.¹¹ MWs may substitute catalysts, in certain reactions, such as in the Kabachnik–Fields condensations of amines, aldehydes and >P(O)H reagents. A series of new α-aminophosphonate derivatives were prepared that displayed significant anticancer activity on certain cell cultures.^{12–14} β-Aminophosphonic derivatives were also prepared and derivatized.¹⁵ The utilization of the Pudovik reaction in the synthesis of α-hydroxyphosphonates and their derivatization,¹⁶ as well as the preparation of hydroxy-methylenebisphosphonates (dronic acid derivatives)¹⁷ as biologically active substrates or drugs in the treatment of bone diseases will also be discussed. Phosphonyl-functionalized hydroxyphosphonates were also synthesized.^{18,19} The hydroxyphosphonates were converted to the mesyloxy derivatives.²⁰ Flow chemical accomplishments of a few reactions mentioned above, *e.g.* esterifications, alcoholyses and hydrolyses are also presented. It is also the purpose of this paper to elucidate the scope and limitations of the MW tool.

Biography:

György Keglevich graduated from the Technical University of Budapest (TUB) in 1981. He got PhD (1984), DSc (1994) and Dr Habil (1995) degrees. He spent his postdoctoral years (1984–85) together with Professor Louis D. Quin (Duke University, Durham, NC, and then University of Massachusetts,

Amherst, MA). He has been the *Head of Department of Organic Chemistry and Technology* for 22 years (1999–2021). He devoted his research career to organophosphorus chemistry developing new synthetic methods and new families of compounds. He also deals with environmentally friendly (green) chemistry embracing MW chemistry, ionic liquids, new catalysts and selective syntheses along with flow chemistry. He took also part in *ca.* 30 pharmaceutical industrial projects developing technologies, whose results were implemented by 3 patents. He is the author or co-author of 699 papers including 42 review articles, 4 books and 55 book chapters. His H index is 48, the number of independent citations is 6591. In the last 5 years, he delivered 16 plenary or key-note lectures. 21 PhD degrees were born with his supervision, 3 degrees are in process.

His educational activity covers delivering lectures in “Organic chemical technology” (both on the BSc and MSc level), “Environmentally-friendly chemistry” (MSc), “Organic chemical basic processes” (BSc/MSc) and “Organophosphorus chemistry”. He directed close to 200 project works and diploma theses.

He is the Editor-in Chief of *Curr. Org. Chem.*, founder E-I-C of *Curr. Green Chem.*, and the Section-E-I-C of the “*Chemical Section*” of *Symmetry*. He is Associate Editor for *Curr. Org. Synth.*, *Lett. in Org. Chem.*, *Lett. in Drug Design and Discovery*, and *Heteroatom Chem.* He is Editorial Board Member for *Molecules* (Green Section), *Green Processing and Synthesis*, and *Phosphorus, Sulfur, Silicon*. He is the member of the *Steering Committee of International Conference of Phosphorus Chem.* (ICPC). The 22. ICPC was arranged in Budapest/Hungary in 2018 under his chairmanship.

Presently, he is the trustee of the Rector in the project “For Green and Sustainable Budapest University of Technology”. He has been acknowledged by the high state decoration of “Knight’s Cross” (2021) and the highest university medal “József Nádor Price” (2022).

Invited Talks

Harvesting Thermal and Mechanical Energy from Environment for Catalytic Applications

Weishu Liu^{1*}, Shun Li²

¹.*Department of Materials Science and Engineering, Southern University of Science and Technology, Shenzhen, China 518055*

².*Institute of Quantum and Sustainable Technology (IQST), School of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang, 212013, China*

Abstract

The thermal and mechanical energy harvesting from environment is a promising solution for the alternative and sustainable energy sources. However, the direct conversion of thermal or mechanical energy to electricity facing the efficiency bottleneck and economic inferior as the energy amount and quality close to waste level. In this work, we present some new insight in exploring the direct coupling of the thermoelectric and piezoelectric effects with catalytic processes, termed as thermoelectrocatalysis (TE-Catal) and piezocatalysis (PZ-Catal), which can be widely applied to a wide range of catalytic applications such as water splitting, organic synthesis, CO₂ reduction, pollutants degradation, and biomedical technologies. Our study focuses on the design of new materials to realize the TE-Catal and PZ-Catal. Regarding the TE-Catal, we summarized and proposed several potential working modes and analyzed the underlying principles of different TE-Catal systems. We also showcase an example of the TE-Catal material, i.e. Bi₂Te₃@MOFs, and present the proposed strategies to improve the catalytic efficiency and stability. For the PZ-Catal case, we systematically investigated the piezocatalytic properties in typical low-dimensional piezoelectric materials (Sr_{0.5}Ba_{0.5}Nb₂O₆, KNbO₃, Bi_{0.5}Na_{0.5}TiO₃, etc.) and revealed the role of critical parameters (e.g., structural characteristics, piezoelectric coefficient and conductivity) in the catalytic efficiency. Our work highlight the feasibility and potential of TE-Catal and PZ-Catal materials could be alternative solution to harness waste energy effectively, thereby contributing to both energy conservation and environmental sustainability.

Biography:

Weishu Liu is a full professor of MSE at Southern University of Science and Technology. He got his Ph.D degree from USTB in 2009, and conducted research at Washington University, Boston College, University of Houston, and Shectak Inc. His research topic is small-temperature-difference thermoelectric conversion materials and novel application. He has published over 160 papers, including Science, Innovation, PNAS, NSR, Energy Environ. Sci., Adv. Mater. etc, with citations over 12000 and H-index of 56. He is a Fellow of the Royal Society of Chemistry, won the first Tencent "XPLOER Award", and "Academic Contribution Award" of Chinese Materials Research Society, C-MRS.

Structural Evolution and CO₂ Electroreduction in Cu-Doped Gold Nanoclusters

Sara Goberna-Ferrón^{1*}, Enric Ibáñez-Alé^{2,3}, Jiajun Hu¹, Josep Albero¹, Carlo Marini⁴, Núria López², Noelia Barrabés⁵, and Hermenegildo García¹.

¹*Instituto Universitario de Tecnología Química (CSIC-UPV), Universitat Politècnica de València, Spain;*

²*Institute of Chemical Research of Catalonia, (ICIQ-CERCA), The Barcelona Institute of Science and Technology (BIST), Spain;* ³*Universitat Rovira i Virgili, Spain;* ⁴*ALBA Synchrotron Light Facility, Spain;*

⁵*Institute of Materials Chemistry, Technische Universität Wien, Austria.*

Abstract

Ligand-protected gold nanoclusters present a promising alternative for electrochemical CO₂ reduction (eCO₂R) due to their enhanced selectivity and tailored composition. This study investigates the influence of different staple motifs in gold nanoclusters (Au₂₅(SR)₁₈ and Au₁₄₄(SR)₆₀) doped with copper (Cu) on their performance in eCO₂R. Detailed cluster characterization and Density Functional Theory (DFT) simulations reveal that ligand dynamics, especially partial removal and staple bending, are critical to understanding the dopant's role and overall catalyst performance. The Cu-doped Au₁₄₄(SR)₆₀ nanocluster demonstrated superior CO production at -0.8 V vs. RHE due to the stabilization of the *CO intermediate, while Cu-doped Au₂₅(SR)₁₈ primarily produced formate but showed lower CO selectivity. These findings highlight the importance of ligand stability and structural dynamics in enhancing the design and efficiency of bimetallic gold nanoclusters for CO₂ reduction.

Biography

Dr. Sara Goberna-Ferrón is a postdoctoral researcher at the Instituto de Tecnología Química (ITQ), Universitat Politècnica de València. She holds a Ph.D. in Nanoscience and Nanotechnology from Universitat Rovira i Virgili. Her research spans catalytic materials, electrocatalysts for CO₂ reduction, and hybrid materials. With extensive international experience, Sara has conducted postdoctoral research in Spain, France, and the USA. She has authored 28 high-quality publications, including a book chapter and a patent, and has an h-index of 18 with over 1400 citations. Sara has presented at numerous prestigious conferences and is passionate about promoting women in science, actively engaging in various outreach activities.

Atom Economical Ni-Catalyzed Reactions of Enynes and Allenynes for the Preparation of Complex Structures (Online)

Diego J. Cardenas*

Departamento de Química Orgánica, Facultad de Ciencias, Universidad Autónoma de Madrid, Institute for Advanced Research in Chemical Sciences (IAdChem), Av. Francisco Tomás y Valiente 7, Cantoblanco, 28049-Madrid, Spain

Abstract

First-row transition metals are becoming more and more important as catalysts for synthetically useful reactions in organic chemistry, replacing the usual heavy-metal catalysts. Nickel is especially interesting for the occurrence of novel activation processes and reaction pathways. We will present the use of polyunsaturated compounds such as enynes and allenynes as starting materials for the development of Ni-catalyzed cascade reactions in which several C-C and C-B bonds are formed in a single synthetic operation, with complete atom-economy and broad scope. Borylative cyclizations lead to the formation of compounds which may be further functionalized. Cycloisomerizations and cyclodimerizations render complex polycyclic products such as ladderanes.

Biography:

Diego J. Cárdenas obtained his PhD at UAM in 1994. After a postdoctoral stay during Louis Pasteur University with Prof. Jean-Piere Sauvage, he joined the UAM where he became Full Professor of the Department of Organic Chemistry in 2010. He has performed two more stays at the U. of Cambridge (2007) and the U. of Michigan (2012). He has worked on organometallic and supramolecular chemistry and currently develops novel high-efficient eco-friendly and economical synthetic methods based on first-row transition metal catalysts, and in the determination of the reaction mechanisms. He has authored over 120 papers and was the Head of the Department of organic Chemistry at UAM (2014-2022).

Exploring Innovations in Ethylene/CO Polymerisation through DFT Calculations: Advancing Sustainable Polymer

Lucia Caporaso*

Department of Chemistry and Biology, University of Salerno

Abstract

More sustainable degradable polyethylene materials have been developed using advanced Ni(II) phosphine phenolate catalysts, incorporating a small amount of carbon monoxide during ethylene polymerization.¹ The isolated keto-units within the polyethylene chains introduce photodegradability, which could help address the environmental persistence of mismanaged polyethylene waste.² The mechanism of this reaction was clarified through a combined theoretical DFT and experimental study using various Ni(II) phosphine phenolate catalysts.³ DFT calculations revealed that the desired non- alternating CO incorporation results from a favorable balance of electronic and steric factors: (I) Moderate steric hindrance from the phosphine moiety promotes the non-alternating pathway. (II) A balanced electronic donation to the electron-poor metal center is necessary to prevent the formation of overly stable chelate species, which, while reducing catalytic activity, would also favor the undesired alternating pathway.

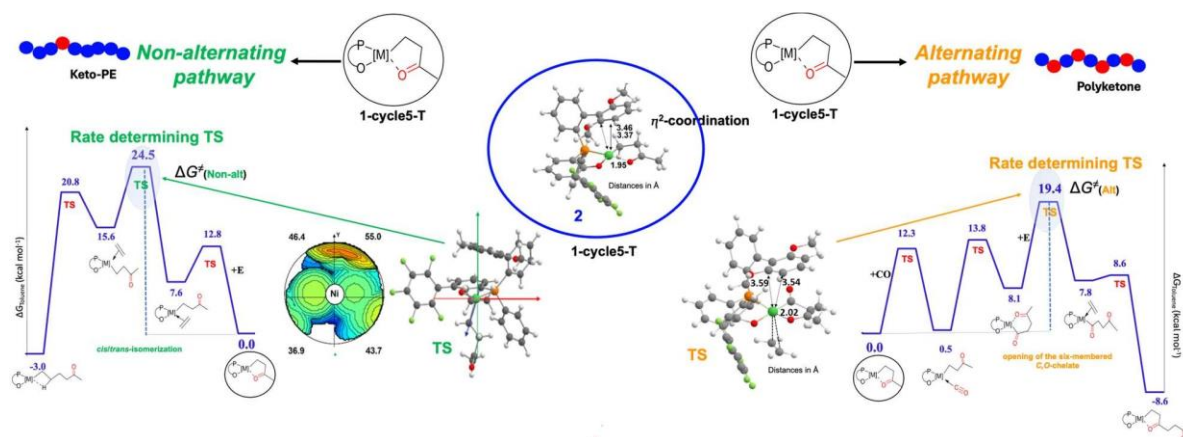


Figure 1. Free energy (ΔG_{TS} kcal mol⁻¹) of key species involved in the formation of Keto-PE (non-alternating pathway) and Polyketone (alternating pathway) from E-CO polymerization with phosphine phenolate catalyst 2.

Innovative Soft-Templating Techniques for Catalyst Synthesis in Anion Exchange Membrane Water Electrolysis

Francisco Fernández-Carretero*, Victor Oestreicher, Immanuel Vincent, Daniela Minudri, Alberto García, Ekain Fernández

TECNALIA, Basque Research and Technology Alliance (BRTA), Donostia-San Sebastián, Spain

Abstract

Anion exchange membrane electrolysis (AEMWE) offers a cost-effective alternative to proton exchange membrane electrolysis (PEMWE) by utilizing more affordable materials. However, enhancing the cycle-life of AEMWE electrolyzers and reducing manufacturing costs are essential for developing a competitive product.

A promising strategy involves the direct synthesis of catalysts on porous transport layers (PTL), eliminating the need for ink or slurry preparation and subsequent deposition. Soft-templating techniques have been successfully applied to synthesize NiS electrocatalysts for hydrogen evolution reaction (HER) under alkaline conditions for AEMWE.

This study employs a molten salt-assisted self-assembly (MASA) process for synthesizing earth-abundant-based electrocatalysts for AEMWE. Catalysts were deposited on PTL substrates via dip coating. Ni sulfides for HER were synthesized, extending the work of Karakaya *et al.* (2020) by examining the impact of varying carbon substrate hydrophobicity. Additionally, for oxygen evolution reaction (OER) catalysts, NiFe catalysts were also synthesized, and the effect of different substrates, particularly the presence of Fe, on electrocatalytic properties was investigated.

Soft-templating methods provide a simple and scalable approach for synthesizing mesoporous catalysts with interconnected electronic and ionic conductive networks, high specific surface area, and improved stability.

This work has been carried out under the frame of the SUSTAINCELL project. The project is supported by the Clean Hydrogen Partnership and its members Hydrogen Europe and Hydrogen Europe Research under Grant Agreement No 101101479.

Biography

Dr. Francisco José Fernández Carretero, (Tecnalia)

Researcher at the department of Hydrogen Technologies at Tecnalia since 2008. Specialising in the development of materials with electroactive properties. His research lines include the development of ion exchange membranes, electrocatalysts and the manufacture of electrodes. His interests include electrolysis, fuel cells and batteries, especially redox flow batteries, metal-air and solid electrolyte batteries.

Session: Photocatalysis and Sustainability

Metal-Organic Framework-Based Photocatalysts for the Generation of Fuels

Amarajothi Dhakshinamoorthy*, Herme G. Baldoví and Sergio Navalón

Departamento de Química, Universitat Politècnica de València, Camino de Vera, s/n 46022, Valencia, Spain.

Abstract

In respect to conventional inorganic semiconductors, metal–organic frameworks (MOFs) have emerged as efficient photocatalysts due to their fascinating physical and chemical properties. MOFs are a class of crystalline porous materials whose crystal lattice is composed of strong coordination bonds between the multitopic organic ligands and metal ions/metal oxo-clusters/metal-oxo chains. Interestingly, MOFs have been reported as one of the suitable (photo)catalysts due to their tunability in the physico-chemical and optoelectronic properties. Thus, the possibility of employing MOFs as photocatalysts has significantly accelerated in the hydrogen evolution reaction using triethanolamine or methanol as sacrificial electron donors. In addition, MOFs have also been reported as photocatalysts for the sustainable conversion of H₂O into H₂ and O₂ assisted by sunlight is increasing considerable interest. Further, CO₂ recycling into fuels is considered as one of the promising approaches to develop a circular carbon economy to achieve carbon neutrality. In this context, photocatalytic CO₂ methanation in the presence of Solar irradiation is appealing technologies for this target.

In the present talk, MOF-on-MOF composites possessing UiO-66 topologies, namely UiO-66(Ce), UiO-66(Zr)-NH₂, UiO-66(Zr)-NH₂@UiO-66(Ce) and UiO-66(Ce)@UiO-66(Zr)-NH₂ are prepared, and their photocatalytic activity is tested in the overall water splitting under simulated sunlight irradiation without any sacrificial agents.¹ Among these photocatalysts, the promising activity is observed with UiO-66(Zr)-NH₂@UiO-66(Ce) photocatalyst exhibiting 708 and 320 μmol g⁻¹ after 22 h for H₂ and O₂, respectively, with 5 mg of solid. Furthermore, it will also be demonstrated that the photocatalytic CO₂ methanation using RuOx supported MIL-125(Ti)-NH₂ allows to operate even under continuous flow operation (> 50 h) and visible light irradiation.²

Biography

Amarajothi Dhakshinamoorthy received his Ph.D., degree in 2009 from Madurai Kamaraj University, Madurai-21, India. Later, he worked as a postdoctoral researcher with Prof. Hermenegildo Garcia at the Technical University of Valencia for four years. Currently, he is working at Departamento de Química, Universitat Politècnica de València, Valencia, Spain as a distinguished researcher. His research interests include (photo)catalytic applications of metal-organic frameworks and graphene-related materials. He has co-authored over 200 publications, six book chapters and one patent. He is also serving as an Early Career Advisory Board member in Molecular Catalysis, Elsevier.

Cement-based materials containing recycled-TiO₂ for photocatalytic applications

Manuel Melero*, Javier Ignacio Carrascosa, Ana Pérez, José Antonio Gómez, Fran Ribes, Ernesto Colomer

Asociación para el fomento de la innovación y sostenibilidad en la Arquitectura, Ingeniería y Construcción (I²CON), Valencia, Spain.

Abstract

Photocatalysis using TiO₂ and light is a promising technique for removing NO_x along with other pollutants, as demonstrated on a laboratory scale. This work focuses on the development and optimization of cement-based materials with enhanced photocatalytic properties through the incorporation of recycled titanium dioxide (r-TiO₂) derived from plastic waste. Initially, the research involved optimizing the material formulations using mortars, followed by validation with concrete mixtures, a fundamental structural material used in various construction applications such as facades, slabs, and furniture, serves as the matrix for these enhanced materials. The aim was to leverage r-TiO₂ to improve the photocatalytic performance of the cement-based materials. The study investigated the effects of different quantities of glass and r-TiO₂ on photocatalytic efficiency and assessed how factors like moisture and irradiation conditions affect the nitric oxide (NO) photoreduction reaction.

Biography:

Manuel Melero, R&D scientist at I²CON brings over 9 years of experience in advanced materials. His career combines both academic and industrial experience, specializing in the synthesis of functional materials and catalysts, as well as in porcelain enamels and organocatalysts, collaborating with institutions such as Vibrantz Technologies and the Chemical Technology Institute (ITQ).

At I²CON, Manuel's research focuses into sustainable construction materials, energy technologies, and circular economy principles. His work involves advancing sustainable concrete formulations, exploring new energy materials, and applying circular economy concepts to material science.

Influence of Surface Microstructure and Molecules on Dynamic Wetting

Yaerim Lee*

The University of Tokyo, Japan

Organic resin and inorganic fiberglass recovery from wind turbine blades using pyrolysis technology

Samy Yousef*

Department of Production Engineering, Faculty of Mechanical Engineering and Design, Kaunas University of Technology, LT-51424 Kaunas, Lithuania

Abstract

The increasing demand for wind energy has generated massive amounts of non-recyclable wind turbine blades (WTBs) that are often disposed of in landfills or incinerated, raising numerous health and environmental concerns. In order to reduce these concerns and enhance the recycling performance of WTBs, this work introduced the thermochemical treatment using pyrolysis process as an environmentally friendly and commercial technology with high conversion rate to recover organic resin in the form of pyrolysis oil and inorganic glass fiber in the form of solid residue product. The conversion was carried out on WTBs made of fiberglass (40 wt.%) reinforced polyester resin (60 wt.%) as a common structure used in wind blades manufacturing in the Baltic region. The experiments were performed via bench-top pyrolysis with 250 g capacity up to 600 °C. The results showed that under the applied pyrolysis temperature, the resin could be converted into styrene (48 %)-rich oil which could be subsequently thermally cracked into value-added aromatic chemicals using different types of zeolite catalysts. While, fiberglass portion remained as a solid residue, it was then subjected to oxidation treatment at 450 °C to remove any other contaminants, thus obtaining pure short fibers that can be used as filler in composite applications.

Biography

Yousef is a chief researcher at Kaunas University of Technology with over seven years of experience in the field of recycling and energy recovery from waste using mechanical, chemical and thermal techniques. He has an extensive academic and research background with 96 papers published in peer-reviewed journals and H-index (35), <https://www.scopus.com/authid/detail.uri?authorId=57202653908>. His research primarily focuses on sustainable industrial technology and clean energy, with a particular interest in catalytic processes, energy recovery, membranes, hydrogen production and its purification. He is a member of COST programme "CA22123" and guest editor of Metals, Materials, and advisory board of Helion Journals.

Oral Presentation

Calcined Titanium-based Organic Framework supported RuO_x nanoparticles as photocatalyst for solar-assisted CO₂ methanation via Sabatier reaction

Marta González-Fernández*,¹, Celia M. Rueda-Navarro¹, María Cabrero-Antonino², Amarajothi Dhakshinamoorthy¹, Belén Ferrer¹, Herme G. Baldoví¹, Sergio Navalón¹

¹*Departamento de Química, Universitat Politècnica de València, Spain;* ²*Instituto de Tecnología Química (UPV-CSIC), Universitat Politècnica de València, Spain*

Abstract

The reduction of CO₂ by sunlight under mild conditions is increasing interest as a research area which can favor decarbonization to produce fuels and chemicals in a circular economy. In this work¹, we report the photocatalytic activity of a series of titanium oxide-based solids prepared by calcination of MIL-125(Ti)-NH₂ decorated with RuO_x nanoparticles (1 wt%) material at temperatures from 350 to 650 °C for CO₂ methanation under simulated sunlight irradiation (45 mW/cm²) at < 200 °C at 1.5 atm total pressure. Among the series of materials, the highest photoactivity activity was achieved by the material synthesized at 350 °C reaching to the production of 4.73 mmol g⁻¹ CH₄ after 22 h and an apparent quantum yield of 0.76, 0.65 and 0.54 % at 400, 500 and 750 nm, respectively, which compares favorably with the activities of other MOF-based materials reported so far^{2, 3, 4}. Electrochemical impedance, electron spin resonance, photoluminescence and *in situ* FT-IR spectroscopies together with transient photocurrent and hydrogen temperature programmed desorption measurements were used to study the possible reaction pathways and the insights into the material's photocatalytic performance. The results of this study showed the possibility of using MOF-based materials as precursors of metal oxide photocatalysts with enhanced activities for CO₂ methanation under sunlight irradiation.

Biography:

Marta González-Fernández was born in Valencia in 1998 and obtained her primary and high school studies in Cartagena, Murcia, Spain. She obtained her bachelor's degree in chemistry from the University of Granada in 2021, and then studied a master's degree in chemistry from the University of Valencia in 2022. Nowadays, she is pursuing her doctoral studied (PhD) in the Department of Chemistry, Universitat Politècnica de València, Spain in the field of photocatalysis by metal organic frameworks and derived materials under the supervision of Prof. Sergio Navalón.

Session: Functional Materials and Physical Chemistry

High Temperature Vacuum Temperature Programmed Desorption as a New Characterization Method for Catalytic Materials

Takeharu Yoshii^{1*}

Tohoku University, Japan

Abstract

Nitrogen (N)-doped carbon materials are attracting attention in the field of catalysis, such as catalysts for oxygen reduction reaction. CHN elemental analysis and XPS were conventionally used for analysis of N species, but their measurement accuracy is approximately 0.1 wt%. Thus, a technique for detailed analysis of N species is desired. Herein, we propose advanced vacuum temperature-programmed desorption (TPD) up to 2100 °C as a new high-sensitivity qualitative and quantitative analytical method for N-doped carbons (Fig. 1a) [1]. In TPD result of N-containing mesoporous carbons, desorption of N-containing gases, NH₃, HCN, and N₂, was observed in a wide temperature range of 300-1900 °C (Fig. 1b). The gas emission patterns obtained by TPD can provide quantitative and qualitative information on the different types of N species including pyrrolic N, pyridinic N, and graphitic N. Furthermore, TPD analysis showed a high quantitative accuracy of the order of 10 ppm (0.001 wt%). The presentation will further highlight broad applications of high-temperature TPD, including analysis of other heteroatoms (hydrogen, oxygen) in catalytic carbon materials [2-4] and N-doped perovskite-type oxides for photocatalysis [5].

Biography:

Takeharu Yoshii (b. 1992) received his Ph.D. degree in Engineering from Osaka University under the supervision of Professor Hiromi Yamashita in 2020. Since 2020, he has been an Assistant Professor at the Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, working with Professor Hirotomo Nishihara. He was conferred the title of Prominent Research Fellow of Tohoku University in 2023. From 2023 to the present, he is participating in the JST PREST "Future Materials" program. His work focuses on the design and synthesis of nanostructured heterogeneous catalysts, and more recently on the development of characterization techniques.

Exploring Ionic Liquid Materials for CO₂ Capture and Utilization: A Journey of Innovation

Marta Corvo*

i3N|Cenimat, Materials Science Dep. (DCM), NOVA School of Science and Technology, NOVA University Lisbon, 2829-516, Caparica, Portugal

Abstract

The current atmospheric CO₂ levels have surpassed the critical 400 ppm threshold. As the most prevalent greenhouse gas generated by human activities and the primary contributor to artificial global warming, the need for CO₂ capture is a pressing global concern. While conventional capture methods focus on solvent scrubbing with chemical absorption of CO₂, they suffer from drawbacks such as solvent loss through evaporation, formation of corrosive byproducts, and high energy consumption during regeneration. This requires us to explore optimized alternatives. Given the scale of global CO₂ emissions, the energy input for recycling capture materials emerges as a pivotal factor that significantly influences the efficiency and cost of the overall process. Ionic liquids (ILs) have been proposed as alternative solvents for CO₂ capture due to their stability and high selectivity. The possibility of manipulating IL properties has made them extremely versatile materials with several applications, from reaction media to catalysis and electrochemistry. The search for superior IL systems has taken us on a journey that started on the optimisation of IL properties for CC, departing to polymeric systems to combine the unique characteristics of ILs with macromolecular frameworks and arriving at aerogels from polyILs (aeroPILs), capable of CO₂ capture and utilization (CCU). This quest has led the design of both the chemical structure and the morphology of materials capable of capturing and performing the CO₂ catalytic conversion [1-4].

Biography:

Marta C. Corvo obtained her degree in Applied Chemistry and a PhD in Chemistry from NOVA University Lisbon, Portugal. She currently leads the Ion Gels team at the Instituto de Nanoestruturas Nanomodelação e Nanofabricação (i3N) at Cenimat, where she is an Associate Researcher. Her research interests encompass ionic liquid and ion gel materials and NMR studies in solid-state and solution. She focuses on various applications such as CO₂ capture and conversion, art conservation, energy, and tissue engineering.

Insights to improve the surface characterisation of porous materials

Ignacio Campello*, Cristina Gutiérrez¹

**,¹ Iberian Centre for Research in Energy Storage (CIIAE), Cáceres, Spain*

Abstract

Studying pore size and surface area is essential for adsorption and catalysis, where outgassing samples is a key step for many textural and surface characterization analysis. Nevertheless, there is a lack of solid publications or studies supporting specific outgassing conditions¹, therefore the applied conditions (temperature & time) are usually remarkably high in order to ensure a complete degasification. This work aims to properly define analysis conditions for standard materials and hereby serve as a base, helping further researchers to set their parameters in order to improve the analysis while saving time and energy. With this regard, Oxygen and Nitrogen isotherms at 77K have been performed to characterize standard materials, such as 13X, Y & 4A Zeolites and AC applying different outgassing conditions. This work demonstrates as well that Oxygen allows a better characterization for standard micro-mesopore structures than Nitrogen at 77K, since Oxygen adapts better to BET theory for its lower quadrupolar moment², reaches smaller porosity and the analysis are faster³, proving that this adsorptive gas is a valid candidate for analysis in porous materials.

Biography:

Ignacio Campello is a researcher at the Iberian Research Centre for Energy Storage (CIIAE). He has a background in Inorganic chemistry and materials science based on CO₂ capture. He has developed industrial experience and expertise in surface chemistry, including sorbent characterisation, gas sorption, heterogeneous catalysis, and activated carbon synthesis. The Iberian Centre for Research in Energy Storage (CIIAE), based in Cáceres town, is a consortium attached to the National Spanish Science Ministry and the National Portuguese Administration. CIIAE pursues research on sustainable energy storage and uses its pilot plant to scale up research from the lab to its final applications.

Surface chemical properties of interstellar grains. Insights from quantum chemical simulations

Albert Rimola*

Departament de Química, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Abstract

The Universe is molecularly rich [1]. Its chemical diversity and complexity are reflected by the almost 300 molecular species detected by rotational emission in the gas phase [2] and the different solid-state phases in the form of refractory dust grains usually covered by ice mantles [3]. The presence of the gas-phase molecules cannot be explained uniquely by reactions taking place in this phase state but chemical reactions occurring on the grain surfaces are essential to rationalize the interstellar chemistry. Traditionally, Astrochemistry has been sustained by combining astronomical observations with astrochemical modelling and laboratory experiments, but this interdisciplinary approach is not enough to fully unveil the grain surface chemistry due to some intrinsic limitations [4,5,6]. Quantum chemical simulations can partly alleviate these limitations as they provide reliable, quantitative atomic-scale information (structure, energetics, and dynamics) of chemical processes taking place on the surface of grains, this way allowing us to determine the actual role of the grains on them. In this contribution, different paradigmatic roles exerted by grains in different chemical reactions of astrochemical interest will be introduced [7,8,9,10], putting special emphasis on their catalytic properties [11,12].

Biography:

Dr. Albert Rimola received his Ph.D. in Computational Chemistry in 2007 from Universitat Autònoma de Barcelona (UAB). He did a postdoc at Univ. Turin simulating the interaction and reactivity of biomolecules with inorganic biomaterials. In 2010 he returned to UAB where he is now Professor at the Dept. Chemistry. His current research line focuses on the computational simulation of surface-induced heterogeneous catalyzed Astrochemistry. Related to this field, he is the PI of Quantumgrain, an ERC Consolidator Grant funded project. He is co-author of more than 150 papers in peer-reviewed international journals.

Rational Design of Electrocatalysts for Maximizing CO₂ Electrolysis Performance

Thuy-Duong Nguyen-Phan*

National Energy Technology Laboratory, 626 Cochran Mill Road, Pittsburgh, PA 15236, USA

Abstract

Electrochemical CO₂ conversion to commodity chemicals, materials, feedstocks, and fuels driven by renewable electricity offers a promising pathway to mitigate the greenhouse effect and reduce global demand for traditional fossil fuels, while simultaneously achieving sustainable energy and carbon neutrality. Since CO₂ electroreduction is highly structure-sensitive, extensive efforts have been devoted to rationally controlling the size, morphology, dimension, chemical composition, surface structure, defects, etc., of the catalysts to improve product selectivity, activity, and durability to approach the feasibility of practical applications (current density higher than 200 mA/cm² and lifetime beyond 1,000 hours).

This presentation will briefly overview diverse research areas of NETL to advance energy and environmental sustainability along with carbon management. Our efforts directly support the US goal of achieving carbon-free power sector by 2035 and net zero emissions by 2050. Subsequently, the talk will primarily discuss how rational design of novel electrocatalysts would maximize the CO₂ conversion in different cell configurations. Numerous spectroscopic, microscopic, and electrochemical characterization tools have been additionally utilized to correlate the structural, physico-chemical, and electronic properties with the activity and selectivity. Our work provides additional design considerations of effective electrocatalysts for industrially relevant CO₂ reduction performance.

Biography:

Dr. Thuy Duong Nguyen Phan is currently Research Scientist at the U.S Department of Energy's National Energy Technology Laboratory (NETL). Her research interests focus on functional materials for energy conversion (carbon capture and conversion, renewable chemicals/fuel production, hydrogen production/utilization), energy storage (battery, supercapacitor, oxygen storage), and environmental sustainability (wastewater/air/metal purification, indoor odor removal, self-cleaning window).

Poster Presentations

From Green Electrons to Molecules: Facilities at Technalia

Victor Oestreicher*

Technalia, Spain

Effect of Cerium Content and Calcination Temperature on the Catalytic Performance of Mg₄Al₂-xCe_x-HT Systems in the n-Butanol Oxidation Reaction

Faiza Sahraoui^{1*}, Naima Haddad¹, Jean-François Lamonier²

¹University of Science and Technology Houari Boumediene (USTHB), Algeria; ²University of Lille, France

Abstract

It is well known that volatile organic compound (VOC) emissions are a major source of air pollution, contributing to the formation of harmful pollutants such as ground-level ozone and PM_{2.5}, and posing serious health risks such as liver damage and cancer. Catalytic oxidation is an effective and low-cost method of decomposing VOCs into harmless carbon dioxide and water. Despite its industrial importance and use as a biofuel, research into the full catalytic oxidation of n-butanol is limited, making it an ideal model VOC for this study aimed at developing highly active catalytic systems for its complete elimination. To exploit the advantages of cerium's oxygen storage capacity and the beneficial properties of hydrotalcites, such as tunable composition, high surface area, numerous active sites and hierarchical pore structures, Mg₄Al₂-xCe_x hydrotalcites (x = 0, 0.4, 2) were synthesised by coprecipitation and calcined at 280°C and 500°C. The obtained materials were characterized by several techniques (XRD, Raman, ATG, BET, and XPS) and were evaluated in the total oxidation of n-butanol at temperatures ranging from 100 to 280°C. The effect of cerium content and calcination temperature on the catalytic performance of these systems was investigated. Preliminary results indicate that increasing cerium content leads significant improvement in catalytic activity, while increasing the calcination temperature does not favor an enhancement in catalytic activity.

Biography:

Mrs Faiza Sahraoui is a doctoral student and member of the research team at the Natural Gas Chemistry Laboratory at the Houari Boumediene University of Science and Technology. She is working on the catalytic oxidation of volatile organic compounds (VOCs), focusing on the development of innovative catalytic systems to effectively eliminate VOCs, thereby contributing to environmental protection and pollution control. Mrs Faiza has published an article in the journal *Catalysts* and is preparing to publish another shortly. She is keen to collaborate with leading experts in heterogeneous catalysis and environmental chemistry to further her academic career.

Functional Gel-Oxalate and Co-precipitation Methods for Methanol and DME Production over Bifunctional CuZnZr-CBV3024E Catalyst

Samira Ebrahimian ^{1,*}

Department of Chemical and Biological Engineering/ Monash University/Australia ^{1,}*

Abstract

Dimethyl ether (DME) production has attracted significant research interest due to its flexibility as a crucial chemical feedstock and a promising, eco-friendly alternative to liquefied petroleum gas (LPG), as well as its potential use as a hydrogen carrier. Cu/ZnO/ZrO₂-CBV3024E (CZZ-CBV) catalysts are well-regarded for their cost-effectiveness and superior catalytic activity in directly hydrogenating CO₂ to DME. This study focuses on synthesizing the CZZ-CBV and CZZ-OX-CBV catalysts using Co-precipitation and Gel Oxalate methods to achieve smaller Cu crystallite sizes and higher Cu dispersion, thereby enhancing catalytic efficiency for CO₂ hydrogenation. Various characterization techniques, including XRD, SEM, BET, H₂-TPR, NH₃-TPD, and TGA, were employed to analyze the catalysts. Catalytic testing was conducted in a fixed-bed reactor (ID= 20 mm, L = 200 mm) at 25 bar and temperatures ranging from 200°C to 250°C. Under T=200°C and P=25 bar reaction condition, the CZZ-CBV catalyst achieved a high DME space-time yield (STY) of approximately 0.16 g/g_{cat}·h over a 4-hour time on stream, with 24% CO₂ conversion and selectivities of 76% CH₄, 23% DME, and 1% MeOH, and no detectable CO formation. The GHSV was 12000 ml/g_{cat}·h with a CO₂/H₂/Ar ratio of 1:3:4. However, using the CZZ-OX-CBV catalyst resulted in different performance characteristics. Initially, it produced more CO via RWGS reaction, and after 4 hours, favorably converted to MeOH, resulting in higher MeOH selectivity (~95%)

alongside low remaining CO and DME. The STY for MeOH was increased to $0.35 \text{ g/g}_{\text{cat}}\cdot\text{h}$, albeit with a lower CO₂ conversion efficiency of 15% compared to CZZ-CBV.

Biography

I am Samira Ebrahimian, a third-year PhD student in the Department of Chemical and Biological Engineering at Monash University, Australia, under the supervision of Prof. Sankar Bhattacharya, Head of the Department of Chemical and Biological Engineering. I am conducting research on CO₂ hydrogenation to MeOH and DME, with a focus on studying the reaction mechanisms. I am utilizing a high-pressure reactor with a larger volume than other reactors reported in the literature and employing various characterization techniques, including SEM, BET, H₂-TPR, NH₃-TPD, DRIFTS, and TGA. Additionally, I have conducted mechanistic reaction studies using the Australian Synchrotron beamline in 2023 and 2024.

CIIAE (Iberian Centre for Research in Energy Storage)

Ignacio Campello*

** Iberian Centre for Research in Energy Storage (CIIAE), Cáceres, Spain.*

Abstract

The aim of this poster is to present and describe the CIIAE (Iberian Center for research in Energy Storage). CIIAE was constituted with the aim to become a global reference in the context of the energy storage cycle, from the initial materials to the scale up of the processes, contributing to the sustainability and decarbonization of the society. CIIAE mission involves research of many different fields related with the energy sector including: Li, Na, Metal-Air batteries, flow batteries, Supercapacitors, Recycling, Hydrogen production, Catalysis fuel synthesis, Electrochemistry, CO₂ capture, thermal storage, atomistic simulations, prototype design, LCA etc. Currently is composed by more than 90 employees including the administrative department and 4 research departments:

- **Pilot Plant:** In charge of design and preparation to scale up research from the lab to its final applications. Pilot plant allows research in initial step to reach a higher degree of development closer to an industrial level.
- **Thermal Energy Storage:** Dedicated to research the storage of energy involving heat transfer. Phase change, thermochemical, integration of thermal systems, prototyping and sorption processes are investigated within the department.
- **Hydrogen and Power-to-X:** Focused on synthesis of fuels, absorption and simulations research. Hydrogen production via electrolysis & photocatalysis, hydrocarbons synthesis integrating CO₂ and hydrogen, gas storage, atomistic simulations and law/policy regulation framework are among the principal interests of the department.
- **Electrical:** Committed to the study and development of batteries, electrodes and their recyclability. Here materials and processes for battery assembly are researched, as well as the cyclability and recycle of the components.

Biography:

The Iberian Centre for Research in Energy Storage (CIAE), based in Cáceres town within the province of Extremadura, is a consortium attached to the National Spanish Science Ministry and the National Portuguese Administration. Founded in 2021, the CIAE emerged as part of Spain's broader strategy to position itself at the forefront of the global renewable energy landscape. CIAE definitive installations are under development and it is composed by 3 buildings: Pilot Plant, Research and Business Incubator. With more than 47.000.000€ of budget, CIAE is committed to play a critical role in supporting European's green energy transition.

Biodiesel Synthesis from date seed oil using camel dung as a novel green catalyst: An Experimental Investigation

Raiedhah A. Alsaiari^a, Esraa M. Musa^a, Moustafa A. Rizk^a

^a*Empty Quarter Research Unit, Department of Chemistry, College of science and art in Sharurah, Najran University, Saudi Arabia*

Abstract

Biodiesel is seen as more environmentally benign than petroleum-based fuels. It is also cheaper and capable of creating cleaner energy, which has a good impact on increasing the bio-economy. An investigation was conducted on a novel heterogeneous catalyst system utilized in the synthesis of eco-friendly biodiesel from date seed oil, a non-edible feedstock obtained through the calcination of desiccated camel manure at varying temperatures. X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET), and scanning electron microscopy (SEM) were utilized to characterize this catalyst. As a result of raising the calcination temperature, the results showed that the pore size of the catalyst decreased. The biodiesel production was optimized to be 86% by using the transesterification method. The confirmation of FAME generation was achieved by the use of gas chromatography-mass spectrometry (GC–MS). The fuel qualities of fatty acid ethyl ester are in accordance with ASTM, suggesting that it is a suitable alternative fuel option.

Keywords: Biodiesel, camel dung, date seeds oil, biofuel, transesterification.

DAY – 3, 04th, October, 2024 - Room A Plenary Speaker

Metal Organic Frameworks as Photocatalysts for the Production of Solar Fuels

Hermenegildo Garcia Gomez*

Polytechnic University of Valencia (UPV), Spain

Biography:

Hermenegildo García Gómez is a full Professor of the Instituto de Tecnología Química at the Univeristat Politècnica de Valencia. His group has expertise in CO₂ utilization developing catalysts for CO₂ conversion to methanol and C₂+ products. He has published over 800 papers, has received over 50.000 citations, has an H index of 110 and his name is included continuously since 2015 in the annual list of the most cited Scientists published by the Shanghai-Tomson Reuters. He is the recipient of the Janssen-Cilag award of the Spanish Royal Society of Chemistry (2011) and the Rey D. Jaime I award in New technologies (2016). He is doctor honoris causa by the University of Bucharest and Honorary Professor at the King Abdulaziz University since 2015. He was awarded by the Lee Hsun lectureship of the Chinese Academy of Science at Shenyang. He has participated in over 20 EU funded projects and is member of the panel of ERC Consolidator Grant as well as other Comissions and panels. He is President of the international advisory editorial board of ChemCatChem. Several of his publications have constituted research fronts in Chemistry (as defined by Essential Science Indicators) Database, such as Photocatalytic CO₂ reduction by non TiO₂ photocatalysis, catalysis by MOFs, etc.

Keynote Talk

Multimetallic Nitrides: Novel, Convenient Synthesis and Electrocatalytic Performance in Water Oxidation Conditions

J.R. Galán-Mascarós, Scott Folkman, F.A. Garcés-Pineda

Institute of Chemical Research of Catalonia (ICIQ-CERCA), Spain

Abstract

In this presentation we will introduce an efficient single-step synthesis of transition metal nitrides (TMNs) using volatile anion salts in anhydrous NH_3 , yielding quantitative amounts of the materials without the necessity for purification steps, while preventing metal-contaminated waste.

Thanks to this novel synthetic protocol, we have been able to access multimetallic nitrides with different stoichiometries, which we have studied as electrocatalysts for water splitting reactions. Our results indicate that mixed metal nitrides of Co, Ni, and Fe outperformed benchmark catalysts for the oxygen evolution reaction (OER), such as IrO_x and also the analogous metal oxides NiCoFeO_x . Incorporated onto gas diffusion electrodes for anion exchange membrane electrolysis (AEMEL). The origin of these high-performances in TMNs resides in their high bulk conductivity (metal nitrides are metallic!) combined with their high electrocatalytic activity developed on their surface, which evolved into the corresponding multimetallic hydroxide layer in working conditions.

Biography:

JR Galan-Mascaros received his PhD in Chemical Sciences from University of Valencia in 1999. After a postdoctoral research stay at Texas A&M University (1999-2001, USA), he joined as “Ramon y Cajal” fellow the Institute of Molecular Science (University of Valencia), where he started his independent career, as I3 researcher, in 2007. In 2009, he moved to the Institute of Chemical Research of Catalonia (ICIQ) in Tarragona, Spain, as ICREA Research Professor and group leader, his current position.

His research career has been essentially multidisciplinary, taking advantage of the tools offered by coordination chemistry to design novel materials for applications in different fields, with particular interest in multifunctional smart materials and solar fuels. He has published over 240 papers, including 10 book chapters; given over 50 plenary and invited lectures; and co-authored over 200 talks and poster presentations in conferences and workshops. He is co-inventor of five patents, and the founder and scientific advisor of the start-up company Orchestra Scientific S.L. His work has been recognized with several awards, including the “Excelencia Investigadora” 2019 award by the RSEQ; the Olivier Kahn international 2008 award by the European Institute of Molecular Magnetism; the “IDEA:Technology” 2006 award by the Fundació Ciutat de les Arts i les Ciències. From 2017 to 2021, he coordinated the European H2020 collaborative project A-LEAF (H2020-FET-PROACTIVE), one of the most important initiative towards the realization of solar fuels.

Iron-Catalysis and their Applications in Synthesis of p-Functional Materials

Rui Shang* and Eiichi Nakamura

Department of Chemistry, The University of Tokyo 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033.

Abstract

As the most abundant metal on Earth with low biological toxicity, iron is ideal as a sustainable catalytic resource for producing organic functional materials. Through years of research on iron catalysis and conjugated materials, we have come to understand various unique properties of organic iron compounds, especially their low oxidation-reduction potentials as catalysts and the mechanism of C-H bond cleavage. The speaker acknowledges that these characteristics give iron catalysis an advantage in synthesizing highly conjugated molecules, especially those with higher HOMO energy levels that are difficult to obtain. We have successfully designed several iron-catalyzed transformations to obtain conjugated molecules, including C-H/C-H coupling for polymerization, tandem cyclization to highly strained frameworks, efficient aza- π extension, and spiro cyclizations. These new methodologies facilitate the efficient synthesis of various conjugated polymers and small polycyclic conjugated molecules. Some new molecules created through our iron catalysis have exhibited excellent performance in solar cells, organic photodetectors, and promising applications for light-emitting diodes, demonstrating the potential for the organic electronics industry.

Biography

Rui Shang is a Professor (特任教授) in the Department of Chemistry at the University of Tokyo. He obtained his B.Sc. and Ph.D. (2014) from the University of Science and Technology of China. He also completed a joint Ph.D. training at the University of Tokyo following a JSPS postdoctoral fellowship (2012-2016) under the supervision of Prof. Eiichi Nakamura. In 2017, he was appointed as a Lecturer at the University of Tokyo, promoted to Associate Professor in 2020, and to Professor in 2024. Dr. Shang's research interests include new catalytic reactions, innovative conjugated molecules, and their material functionalities. He has been recognized with several accolades, including the 100 Excellent Doctor Thesis Award from the Chinese Academy of Sciences in 2015 and the Springer Doctoral Thesis Prize in 2016. Additionally, he was appointed as an Early Career Advisory Board member for the Science of Synthesis (SoS) and a JSP fellow at the B \ddot{u} rgenstock Conference in 2022. In recognition of his contributions, Dr. Shang has received the Banyu Chemist Award in 2022, the Young Chemist Award of the Chemical Society of Japan in 2022, and the Thieme Chemistry Journals Award in 2023.

Session: Catalytic reaction engineering

Chemoenzymatic Cascade Reaction for The Synthesis of High Value Products

Ryszard Ostaszewski*

*Institute of Organic Chemistry of Polish Academy of Sciences, Poland, 01-224 Warsaw, Kasprzaka
44/52*

Abstract

The multistep syntheses of molecules require sequential isolation, purification, and characterization of intermediates and are associated with high solvent, chemical, and energy consumption. The synthesis of stereoisomerically pure products is even more challenging since additional resolution of intermediates into single stereoisomers is required, which complicates and elongates synthetic procedures. In this respect, the cascade reactions that comprise at least two consecutive reactions such that each subsequent reaction occurs only in virtue of the chemical functionality formed in the previous step become of great importance. In cascade reactions, isolation of intermediates is not required, as each reaction composing the sequence occurs spontaneously.

Biocatalytic protocols are a green alternative to chemical processes because enzymes can catalyze numerous reactions under very mild conditions with high selectivity. Therefore, their use in organic synthesis is still being considered as an attractive alternative to classical chemical approaches. For the synthesis of complex chiral molecules, the chemoenzymatic cascades can be used, combining the productivity of different catalysts (i.e. metal-catalysts and biocatalysts), enabling the realisation of a one-pot, multi-step procedures with one catalytic system, avoiding the isolation and storage of unstable or toxic reagents. The presentation will focus on the development of different chemoenzymatic cascade strategies involving Ugi and Passerini reactions for peptidomimetic syntheses, sequential DKR-RCM protocol for syntheses of enantiomerically pure lactones, Knoevenagel condensation leading to isomerically pure product, and chemoenzymatic paraquinols syntheses. The role of enzymes will be highlighted and the perspective of possible applications will be discussed.

Biography

Ryszard Ostaszewski graduated from Warsaw Technical University and then moved to the Institute of Organic Chemistry of the Polish Academy of Sciences, where he obtained his academic degrees; Ph.D. in 1989, D.Sc. in 1999, and Professorship in 2009. From 2009 he holds a position of Full Professor at Institute of Organic Chemistry PAS. His scientific interests comprise the chemistry and stereochemistry of multicomponent reactions, biocatalytic syntheses of enantiomerically pure peptidomimetics, enzyme immobilization, and domino/cascade chemoenzymatic processes. He is the author or coauthor of over 150 publications, including one chapter in a book.

Activity and Stability of Hybrid Polyoxometalate-layered Double Hydroxide Nanocomposites Under Electrocatalytic Water Oxidation Conditions

Joaquín Soriano-López^{1*}, Javier Quirós-Huerta¹, Álvaro Seijas-Da Silva¹, Ramón Torres-Cavanillas¹, Eduardo Andres-García¹, Gonzalo Abellán¹ and Eugenio Coronado¹

¹*Institut de Ciència Molecular, Universitat de València, Catedrático José Beltrán², 46980 Paterna, Spain*

Abstract

Polyoxometalates (POMs) have been thoroughly studied as oxygen evolution reaction (OER) materials, whereby structure/activity relationships have provided knowledge to rationally design POMs with increased catalytic capabilities.[1] Heterogenization of POMs is a promising strategy to increase their OER activity and to overcome stability issues seen under homogeneous conditions.[2] A common heterogenization approach is the deposition of POMs over the positively charged surface of bulk materials via electrostatic interactions. 2D materials offer an appealing platform to obtain hybrid nanocomposites with monodisperse POMs over the 2D surface. In this respect, layered double hydroxides (LDHs), formed by positively charged brucite-type inorganic layers stacked together with interlayer anions forming sandwich structures, are 2D materials with applications in different energy-related areas.[3] POMs, as polyanionic species, are excellent candidates to be combined with LDHs to obtain hybrid POM/LDH nanocomposites. These nanocomposites have been typically employed as catalysts for fine organic synthesis.[4] However, only a few examples of their use as OER materials are reported in the literature, in which the fate of the POM counterpart under working conditions has not been properly established.[5] Here, I will present our most recent results on the OER activity and stability of hybrid POM/LDH nanocomposites.

Biography:

Dr. Joaquin Soriano-Lopez holds an MSc in Synthesis and Catalysis (2013) and a PhD in Science and Chemical Technology (2016) from the Catalan Institute of Chemical Research and the Universitat Rovira i Virgili, where he conducted research under the guidance of Prof. José Ramón Galán-Mascarós and Prof. Josep M. Poble.

In 2016, Dr. Soriano-López began his postdoctoral career in Prof. Poble's group at Universitat Rovira i Virgili, before joining the group of Prof. Wolfgang Schmitt at Trinity College Dublin in 2017. In 2021, he was awarded a CDEIGENT fellowship under the Valencian Plan GenT of Excellence, enabling him to join Prof. Eugenio Coronado's group at the Institute of Molecular Science, Universitat de València.

His research focuses on advancing the understanding of metal-oxide nanoclusters, metal-organic frameworks, and 2D materials as water oxidation catalysts. By exploring the structure-reactivity relationships of these catalysts, Dr. Soriano-Lopez aims to facilitate the rational design of more efficient and durable materials. His work has made significant contributions to the scientific community by enhancing the understanding of the complex water oxidation reaction and providing novel insights into the chemical design of materials with improved catalytic performance and stability.

Coal fly ash and acid mine drainage-based Fe-BEA catalysts for the Friedel-Crafts alkylation of benzene.

Tapiwa Hlatywayo¹, Leslie Petrik^{1*}, Benoit Louis²

¹University of the Western Cape, Republic of South Africa; ²University of Strasbourg, France

Abstract

Coal fly ash and acid mine drainage are significant environmental issues in South Africa, causing storage constraints and impacting water quality. This study explores the use of coal fly ash and acid mine drainage in preparing zeolite HBEA-supported Fe catalysts. The catalysts were synthesised using coal fly ash as a feedstock for zeolite synthesis, followed by hydrothermal treatment. The Fe was loaded to the zeolite using liquid phase ion exchange and wet impregnation, with acid mine drainage as the metal solution precursor. The Friedel-Crafts alkylation of benzene with *t*-butyl chloride was used as a probe reaction. The highest *t*-butyl chloride conversion of 100 % was obtained over the ion exchanged 25AHI catalyst after 0.5 hours onstream, while the highest selectivity towards formation of *t*-butylbenzene was achieved over the wet impregnated 25AHW catalysts after 0.5 hours on stream. The study also found that other metals present in AMD affected the overall activity, with Ni having a positive effect on the conversion and selectivity while, Mn, Ca, Mg, and Na had a negative effect on the conversion chloride but a positive effect on the selectivity towards formation of the monoalkylated (*t*-butylbenzene). This study demonstrates that green solid acid catalysts with high catalytic activity can be prepared using two waste materials, coal fly ash and acid mine drainage. To the best of our knowledge we are reporting for the first time, the use of acid mine drainage as a metal precursor in catalyst preparation.

Biography

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Oral Presentation

Innovative Flow-Cascade Process for Amino-Ester Production from Biomass Platform Molecules

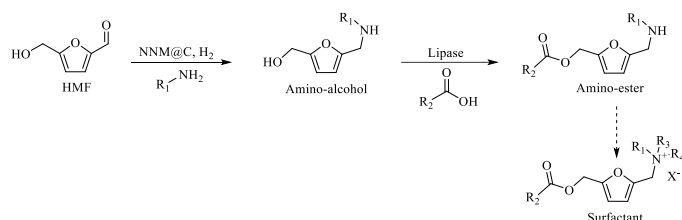
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Abstract

Biomass, along with CO₂, represents the only alternative carbon source to fossil fuels. Biomass valorization into high-value chemicals and biofuels can be achieved by transforming so-called platform molecules. Among them, 5-hydroxymethylfurfural (HMF) is one of the most important molecules due to its high functionality, allowing it to be converted into a wide variety of high-value derivatives [1]. Among these derivatives, N-substituted furfurylamines, which can be synthesized through the reductive amination of HMF [2], are an important class of compounds due to their pharmaceutical applications and as intermediates in the synthesis of surfactants based on quaternary ammonium salts [3].

In this work, amino-esters derivatives of HMF, useful as precursors of ammonium salts surfactants, have been synthesized through a chemo-enzymatic cascade process in continuous flow reactors by coupling of the reductive amination of HMF with primary or secondary amines, followed by selective esterification of the hydroxymethyl group of the resulting amino-alcohol with fatty acids, using a supported lipase (CALB) as a biocatalyst (Scheme 1).



Scheme 1. Cascade process for surfactant synthesis from HMF.

For this purpose, the reductive amination of HMF with different primary and secondary amines was first optimized using cobalt nanoparticles encapsulated in carbon as a hydrogenating catalyst (Co@C) [4]. Optimization of the enzymatic esterification stage, allowed us to perform the chemo-enzymatic process by coupling both steps in two continuous flow reactors achieving the target amino-esters in excellent yields and high chemoselectivity.

Invited talk

Phosphine-Driven Near UV Photoinitiation for User-Friendly Peptide and Desulfurization

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Abstract

Peptides are increasingly important as pharmaceutical targets, necessitating efficient, green synthesis methods. A key limitation is the lack of an industrially viable peptide desulfurization technique, essential for native chemical ligation in drug production. Current methods require large amounts of reagents or rare catalysts. We present a phosphine-only photodesulfurization (POP) using near-UV light that is clean, high-yielding, and requires minimal phosphine. This userfriendly reaction works in various solvents, on protected/unprotected peptides, and on a gram scale, preserving sensitive functional groups. POP's utility is demonstrated on cyclic peptides, GLP-1, linaclotide, and wheat protein.
