



**II WORKSHOP ON MATERIALS FOR PHOTOCATALYSIS
FOR ENERGY AND CLEAN ENVIRONMENT”**

University of La Laguna, Tenerife. February 22nd – 23rd, 2024

Acknowledgements

The organizing and scientific committee of the “II Workshop on Materials for Photocatalysis, Energy and Clean Environment” would like to express its gratitude to the public institutions and private companies that have sponsored this event. The IWMPECE would not have taken place successfully without their sponsorship and support.

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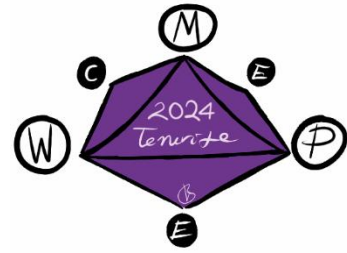
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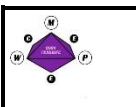


The first workshop, “Workshop on Photocatalysis for energy and Clean Environment”, was held in October 2022 at the University of Malaga, and organized by Professor Enrique Rodríguez Castellón. The first Workshop was focused on photocatalysis and its applications. In this second workshop we have extended the topics to materials for photocatalysis, green energy and a clean environment, as indicated in the title.

The “II Workshop on Materials for Photocatalysis, Energy and Clean Environment” has a higher participation with +50 participants presenting abstracts, being +35 from outside Tenerife, including 7 different nationalities. The scientific level of the abstracts is indicative of the high expected quality of oral and poster presentations on the workshop topics.

The Organizing and Scientific Committee of the IIMPECE would like to thank all the participants and attendees of this workshop. Especially scientists and students, who have come from abroad and other parts of Spain research centers, as well as the students from the University of La Laguna for their massive turnout. All of them specialized in the topics of the workshop and concerned about clean and green energy and keeping the planet sustainable for future generations.

The Organizing and Scientific Committee of II Workshop
on Materials for Photocatalysis, Energy and Clean
Environment (II WMPECE).



OVERALL PROGRAMME

II Workshop on Materials for Photocatalysis,
Energy and Clean Environment (IIWMPECE).

	Thursday 22 nd February 2024	Friday 23 rd February 2024
08:30 - 09:00	Presentación	
09:00 - 09:45	Teófilo Rojo	Ana Belén Jorge Sobrido
09:45 - 10:15	Elisa Moretti	Marcos Fernández-García
10:15 - 10:45	Conchi Ania	Anna Kubacka
10:45 - 11:15	Federico Polo	Javier Fernández Sanz
11:15 - 11:45	Coffee break	Coffee break
11:45 - 12:00	Gerardo Colón	Sergio Díaz Coello
12:00 - 12:15	Juan Carlos Colmenares	Yolanda Pérez Cortés
12:15 - 12:30		Giada Caniglia
12:30 - 12:45		Gustavo J. Chacón Rosales
12:45 - 13:00	Domingo Pérez Coll	Hakim Faraji
13:00 - 13:15	Jesus Prado Concal	Closing Ceremony
13:15 - 13:30		
13:30 - 13:45		
13:45 - 15:30	Lunch and Poster Session	Lunch and Poster Session
15:30 - 16:00	Elena Pastor	Excursion to the base of the Volcano "El Teide" visit to the Astronomical Observatory of Izaña, (Astrophysics Institute of Canary Islands) followed by a wonderful sunset viewing. gala dinner in Las Cañadas del Teide (at an altitude of 2150m.), night vision of the stars with specialists after dinner Scheduled to return at midnight to La Laguna
16:00 - 16:30	Alfonso Caballero	
16:30 - 17:00	Luis Sánchez Granados	
17:00 - 17:30	Coffee break	
17:30 - 17:45	Juan Carlos Calderón	
17:45 - 18:00	Orhan Sisman	
18:00 - 18:15	Ricardo A. Medina Echevarria	
18:15 - 19:15	Flash Oral Session	
19:15 - 20:00	Poster Session	

PROGRAMME OF II WMPECE

22nd February 2024

8.30 Aperture

Prof. Antonio Aparicio, Vice-Rector for Research (ULL)

Prof. Pedro Núñez Coello (Chairman)

Prof. Enrique Rodríguez Castellón (Co-Chairman)

Session Chairperson: Enrique Rodríguez Castellón

9:00 Teófilo Rojo, University of Basque Country

"Advanced Materials for Li and Na-ion battery technologies: Effect on the energy transition."

9:45 Elisa Moretti, Ca' Foscari University of Venice

"Customizing inorganic nanomaterials synthesis for environmental remediation."

10:15 Conchi Ania CEMHTI (UPR 3079), CNRS, Univ. Orléans, Orléans, France

"Applying photocatalysis to the regeneration of saturated granular activated carbon used in water treatment: a pilot scale study."

10:45 Federico Polo, Ca' Foscari University of Venice.

"Nickel Hexacyanoferrate Nanocubes as Highly Performing Catalyst for Solar-Light-Driven Photodegradation of Metronidazole."

11:15 Coffee break

Session Chairperson: Elena Pastor Tejera

11:45 Gerardo Colón Institute of Materials Science Seville, CSIC

"Thermal Assisted Photocatalysis for Energy Applications: H₂ Production and CO₂ Valorisation."

12:15 Juan Carlos Colmenares Polish Academy of Sciences

"Carbon-based nanostructured composite (piezo)photocatalysts: energy and organic redox synthesis applications."

12:45 Domingo Pérez Coll, Institute of Ceramic and Glass-CSIC, Madrid

"Layered cathode architectures deposited by spray pyrolysis for optimized solid oxide cells."

13:15 Jesús Prado Concal, Complutense University of Madrid

"Harvesting power from waste heat: Unveiling the potential of thermoelectric materials for clean energy generation."

13:45 Lunch and Poster Session

Session Chairperson: María del Carmen Román

15:30 Elena Pastor Tejera, University of La Laguna

"Noble metal-free catalysts for electrolysers and fuel cells."

16:00 Alfonso Caballero Martínez, University of Sevilla

“Cobalt-based Mesoporous TiO₂ Catalyst for Fischer-Tropsch Reaction.”

16:30 Luis Sánchez Granados, University of Cordoba

“2D/2D NiTi-LDH/BiOBr photocatalyst with extraordinary NO_x removal under visible light.”

17.00 Coffee break

Session Chairperson: Juan Carlos Colmenares

17.30 Juan Carlos Calderón, University of La Laguna

“Modification of nanostructured materials with natural dye sensitizers: applications in energy production and water electroremediation.”

17.45 Orhan Sisman, Alexander Dubček University of Trenčín, Slovakia

“Photocatalytic activity of TiO₂ nanorods on spherical FTO granules”

18:00 Ricardo Adolfo Medina Echavarría, University of Manizales (Colombia)

“Design of a solar cell based on simulations of InAlN semiconductor nanostructures.”

18.15 Flash Oral Session

Flash Communication Session Panel:

Enrique Rodríguez Castellón, Ana Belén Jorge Sobrido,

Alfonso Caballero and Conchi Ania

18.15 Abraham Castilla Silvestre, University of La Laguna

“Unleashing the potential application of direct ammonia fuel cells”

18.20 Stephan Delgado, University of La Laguna

“MXenes as catalysts for hydrogen evolution reaction”

18.25 Modesto González Rodríguez, University of La Laguna

“La_{3-x}Ca_xNbO_{7-δ} for application in power conversion devices”

18.30 Hans Klein Sánchez, University of La Laguna

“Zn_{1-x}Cd_xS/TaON for photocatalytic water splitting”

18.35 Jesús Gabriel Madrid Negrín, University of La Laguna

“Electrolytes with pyrochlore structure based on the La_{2-x}Ca_xScNbO_{7-δ} for application in solid oxide electrolyzers (SOEC)”

18.40 María Luisa Marín Universidad Politécnica de Valencia

“Photocatalysts for environmental applications”

18.45 Airán Ródenas, University of La Laguna

“reactor: Optical fibre plasmonic microreactor for flow chemistry”

18.50 Víctor Sánchez Toledo, University of La Laguna

“Heterostructures of β-TaON with TiO₂ for hydrogen production by water splitting”

19.15 Poster Session

20.00 End of day

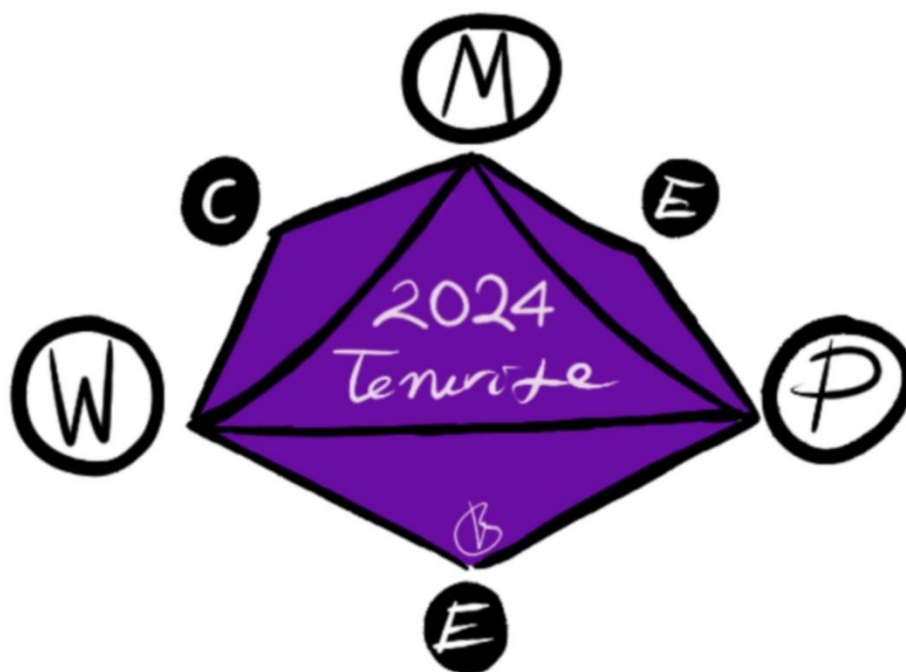
23rd February 2024

Session Chairperson: Gonzalo García Silvestro

- 9:00 Ana Belén Jorge Sobrido, Queen Mary University of London**
"Modifying hematite to enhance photoelectrocatalytic activity for water oxidation."
- 9.45 Marcos Fernández-García, Institute of Catalysis and Petrochemistry- CSIC, Madrid**
"Photocatalysis: Quantitative analysis of Photo and Thermo-Photo Reactions "
- 10:15 Anna Kubacka, Institute of Catalysis and Petrochemistry – CSIC, Madrid**
"Photo and Thermo-Photo Production of Hydrogen from biomolecules."
- 10:45 Javier Fernández Sanz, University of Seville**
"High-throughput screening of thermoelectric materials by machine learning "
- 11:15 Coffee Break**

Session Chairperson: Elisa Moretti

- 11:45 Sergio Díaz Coello, University of Innsbruck**
"Alkaline CO reduction at modified Cu single crystals - Chasing the selective formation of ethanol."
- 12.15 Yolanda Pérez Cortés, IMDEA- Rey Juan Carlos University**
"Improved Photocatalytic Performance of Lead-Free Organic-Inorganic Hybrid Perovskites in H₂ Production. "
- 12.30 Giada Caniglia, Ulm University**
"Investigation of nano- and micro-photocatalytic systems via scanning electrochemical probe microscopy."
- 12.45 Gustavo Javier Chacón Rosales, Polytechnic University of Valencia-ITQ**
"Advancing Hydrogen Production: Exploring Alcohol Photo Reforming with Hybrid Gold Based Catalysts Generated Through Physical Enrichment."
- 13.00 Hakim Faraji, University of La Laguna**
"Covalent Triazine Frameworks for Photocatalytic Applications: challenges and new opportunities. "
- 13:15 Closing ceremony**
- 13.45 Lunch**
- 15.15 Tour to El Teide.**



**ORGANIZING AND SCIENTIFIC
COMMITTEE OF THE
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Pedro Núñez Coello University of La Laguna



Pedro Núñez, is currently full professor at Department of Inorganic Chemistry at University of La Laguna, where he is the leader of the research group “Ceramic Materials and SOFCs. His research is devoted to materials for a clean and sustainable energy. Especially in ceramic materials for energy, focused on the development of electroceramics for IT-SOFC, including proton and oxide conductors. Also, on ceramic materials for photocatalytic applications, such as green hydrogen production via water splitting.

Enrique Rodríguez Castellón University of Málaga



Enrique Rodríguez Castellón is full professor at the University of Málaga and President of the Inorganic Division of the Royal Society of Chemistry of Spain. He has more than 45 years of experience in teaching and researching. He has published more than 630 scientific papers, 36 book chapters and 8 patents. More than 20.000 citations and $h = 65$ (SCOPUS). He has participated in 7 European Projects, 37 national and regional projects and 20 contracts with different water and energy companies. He is specialist in materials science, environmental catalysis, adsorption with special interest in CO_2 capture, H_2 generation and purification, X-Ray photoelectron spectroscopy and wastes valorization. He is Doctor Honoris Causa by the Federal University of Ceará (Brazil).

Elena Pastor Tejera University of La Laguna



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



Gonzalo García Silvestro *University of La Laguna*

Gonzalo García is associate professor at the University of La Laguna, deputy director of the Institute of Materials and Nanotechnology, founding and scientific coordinator of the Network of Argentine Scientists in Spain and founding partner of Materials Invisible to Oxygen S.L. His research interests are in fundamental and applied studies of (photo)electrochemical and (photo)electrocatalytic processes. García's leading role in the field of interfacial (photo)electrochemistry and (photo)electrocatalysis is demonstrated by some 88 articles, 8 book chapters, 1 book, 5 patent applications (2 granted), 31 inter/national research and industrial projects (9 as Coordinator (IP)).



Juan Carlos Calderón Gómez *University of La Laguna*

Juan Carlos Calderón is contracted researcher "María Zambrano" at University of La Laguna. His area of expertise is the electrochemistry, mainly applied to the design of novel materials with potential applications in energy production and storage. His experience includes different postdoctoral contracts in prestigious universities and research institutes where he developed materials to produce clean energy, including their physicochemical and electrochemical characterization. The results of his research have been published in high impact factor journals, contributing in this way to the search of materials with outstanding properties in the field of renewable energy.



Modesto González Rodríguez *University of La Laguna*

Modesto González is PhD student at the University of La Laguna. Graduate in chemistry from the University of Laguna and holds a master's degree in molecular nanoscience and nanotechnology. His doctoral thesis focuses on the study of advanced ceramic materials with proton conductivity with application in energy conversion devices. His main interests range from structural determination by x-ray and neutron diffraction, as well as the determination of electrical properties by complex impedance spectroscopy.



Hans Klein Sánchez *University of La Laguna*

Hans Klein obtained the degree on Chemistry (2022) and the M.Sc. (2023) in organic chemistry by University of La Laguna. Currently working as intern researcher at Institute of Materials and Nanotechnology at the University of La Laguna, Tenerife. The main studies focus on the development of materials for green hydrogen production by photocatalytic water splitting.



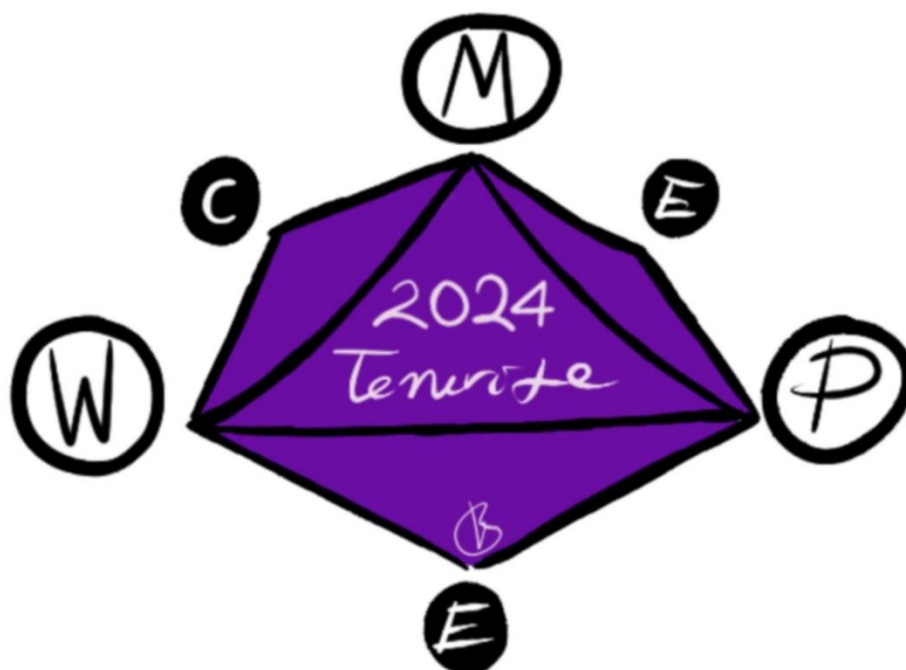
Jesús Gabriel Madrid Negrín *University of La Laguna*

Jesús Gabriel Madrid is a student at University of La Laguna. He's currently studying the MSc. of Molecular Nanoscience and Nanotechnology. He has worked with proton conducting ceramic materials through his TFG and now during his TFM in the group of Dr. Pedro Núñez. He has great interest in materials science and inorganic chemistry.



Víctor Sánchez Toledo *University of La Laguna*

Víctor Sánchez is an undergraduate student at the University of La Laguna. He's currently finishing his bachelor thesis about new materials for photocatalytic water splitting. Víctor also won a third prize in poster communication in the XVII CESQUIM. He also participated in an Erasmus stay at the University of Gdansk (Poland).



**GUEST AND ORAL
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Teófilo Rojo Aparicio University of Basque Country



Teófilo Rojo has been full professor of Inorganic Chemistry at the University of the Basque Country (UPV-EHU) since 1992. His research is focused on energy storage systems (batteries and supercapacitors). From 2010 to 2020, he has been the scientific director of the CIC energiGUNE. He was awarded with the National Prize in Inorganic Chemistry by the RSEQ in 2013. He was appointed as a correspondent academic member of the Royal Spanish Academy of Exact, Physical and Natural Sciences in 2015. He was a member of the Executive Committee of the Division of Solid-State Chemistry and Materials (DSSMC) from EuCheMS (2014-2016) and in 2016, he was appointed as a member of the Chemistry and Energy of EuCheMS (European Chemical Science). He was Highly Cited Researcher in the field of Cross-Field 2021 and in the field of Environment and Ecology 2022.

Ana Belén Jorge Sobrido Queen Mary University of London



Ana Belén Jorge Sobrido did her undergraduate in Chemistry at the University of La Laguna, followed by a PhD at the Materials Science Institute of Barcelona, and a short postdoc back to the ULL before conducting a 5-year postdoc at University College London. In 2016 she joined Queen Mary University of London as academic fellow. Since 2023, she is a professor of Sustainable Energy Materials and UKRI future leaders fellow. Her research focuses on designing new energy materials and gaining deeper understanding of structure-property relationships in energy conversion and storage technologies.

Conchi O. Ania CEMHTI-CNRS Orleans



Conchi Ania received her PhD degree in 2003 (Oviedo, Spain) and performed postdoctoral stays in USA and France. In 2009 she became tenured scientist at Agencia Estatal CSIC, and in 2017 she joined CNRS as directrice de recherche. She held an ERC-Consolidator grant (2016-22) for investigating photochemistry of carbon materials. In 2023 she has received the Silver Medal of CNRS. She is editor of Carbon journal since 2020 (Elsevier).



Alfonso Caballero Martínez *University of Seville*

Alfonso Caballero 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 NO_x 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 within the framework of research projects financed by the Spanish Ministry of Science, International cooperation, European and regional projects, as well as R+D+i contracts and service provision contracts with different companies.

Juan Carlos Colmenares Quintero *Polish Academy of Sciences*



Juan Carlos Colmenares is a full professor at the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC-PAS). He is a Marie Skłodowska-Curie fellow. He graduated from the Warsaw University of Technology (1995), obtained his M.Sc. (1997) in catalysis, and got his PhD (2004) in chemistry from the Warsaw University of Technology. He then worked at the University of Cordoba (2005–2006) and later at the University of Southern California (2006–2009) in Prof. George Olah's (Nobel Prize in Chemistry) group. He received his habilitation (D.Sc.) in 2015 from IPC-PAS, and in 2023 full professor in Chemical Sciences.

Gerardo Colón *Institute of Science of Materials of Seville*



Dr. Gerardo Colón was born in Seville, Spain. He received his BS degree in Chemistry (1992) and PhD degree (1996) from the University of Seville. Between 1996–1998 he worked as a postdoctoral fellow at the Università degli Studi di Cagliari (Italy) and Ecole Supérieure des Mines de Saint Étienne (France). From 2010 Scientific Researcher of CSIC at the same Institute. His research is mainly focused on the development of highly photoactive catalysts for energy and environmental applications. He has published 138 scientific papers ($h = 55$) with more than 10100 citations.



Sergio Díaz Coello *University of Innsbruck*

Sergio Díaz Coello is a researcher at the University of Innsbruck, Austria. He obtained his PhD in Chemistry at the University of La Laguna in 2023, presenting a dissertation on cathodic catalysts for application in alkaline water electrolysis (grading *cum laude*). Currently, he is still working in the field of electrocatalysis, but focusing on the generation of valuable chemicals from CO₂/CO using copper surfaces



Marcos Fernández García *Institute of Catalysis and Petrochemistry*

Marcos Fernández García is Research Professor at the Institute of Catalysis and Petrochemistry (CSIC) and Associate Editor of Applied Catalysis A: General. The main scientific output corresponds to 3 (edited) books, 25 book chapters, 9 patents, and ca. 300 SCI-JCR published works, rendering a Hirsch index of 70 and summing, according to Scopus, > 20.000 citations.



Javier Fernández Sanz *University of Seville*

Javier Fernández Sanz is full professor of Physical Chemistry at the University of Seville, Spain. Member of the Royal Academy of Sciences of Seville. Citation h-index: 49 (WoS). Total citations > 8.500, > 225 papers in refereed journals. Main research interests fall within the Computational Materials Science general topic and can be broadly described as the development and application of methods and models to simulate material properties and surface reactions using quantum mechanical theory and statistics. In particular, structural and electronic properties of a variety of materials, such as metal-oxides, metal/metal-oxide interfaces, and mixed metal-oxides nanostructures.



Anna Kubacka *Institute of Catalysis and Petrochemistry*

Anna Kubacka is a tenured scientist at the Institute of Catalysis and Petrochemistry, CSIC. The main scientific output corresponds to 8 book Chapters, 10 patents and ca. 150 SCI-JCR published works with a Hirsch index of 48. She has served as editor on several special issues on leading journals of the field of Catalysis as well as a member of the editorial board of journals such as Catalysis and Frontiers in Chemistry.



Elisa Moretti *Ca' Foscari University of Venice*

Elisa Moretti (EM) is associate professor of Inorganic Chemistry at the Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice (Italy). She is leading a multidisciplinary team on 0-2D inorganic nanomaterials with tunable size, morphology, porosity, and crystalline phases, for environmental and energy-related applications. Since 2024 EM is chairholder of a UNESCO Chair on Technologies and Materials for Green and Energy Applications (AID4GEA). EM is founder and scientific supervisor of the spinoff ChEERS - Circular Economy for Energy Recycling Solutions, working on a sustainable upcycling and valorization of industrial and agri-food wastes.



Domingo Pérez Coll *Institute of Ceramic and Glass*

Domingo Pérez Coll is a tenured scientist at the Institute of Ceramics and Glass (Spanish National Research Council), in Madrid. His main interests focus on inorganic oxides for electrical and electrochemical applications at high temperature. In particular, he has been researching solid oxide fuel cells and electrolyzers for over 20 years, from the synthesis and design of components to the implementation and characterization of lab-scale device



Jesus Prado Gonjal *Universidad Complutense de Madrid*

Dr. Jesús Prado Gonjal is an Associate Professor in the Department of Inorganic Chemistry at University Complutense of Madrid. He previously worked in the Solid-State Chemistry group at the University of Reading and in the 2D-Foundry group at ICMM-CSIC. His research is focused on studying the relationship between synthesis, structure, and properties of new materials for energy applications, including thermoelectrics, solid oxide fuel cells (SOFCs), and next-generation batteries.



Luis Sánchez Granados *University of Córdoba*

Luis Sánchez is full professor of the Inorganic Chemistry Department of the University of Córdoba. His scientific activity has been carried out mostly in the field of study of solid-state chemistry. On the last 12 years, he is mainly working in the study of new photocatalytic materials for De-NO_x actions. Overall, his scientific activity is summarized by the publication of 120 papers and 140 communications presented at national/international congresses (h index = 37).



Giada Caniglia *Ulm University*

Giada Caniglia completed her Bachelor's (2016) and Master's (2017) in Chemistry at University of La Laguna. After her master's, she worked for 6 months at the Electrochemistry and Corrosion Group of the same university, focusing on the study of corrosion processes using scanning electrochemical microscopy. From 2019 and 2023 she worked as a doctoral student at the Institute of Analytical and Bioanalytical Chemistry (Ulm University), under the supervision of Prof. Christine Kranz and worked on developing and investigating antimicrobial systems via scanning probe techniques. Since 2023 she is a post-doc at the same institute focusing her research on molecular light-driven catalysis using scanning probe microscopy techniques.



Gustavo Chacón Rosales *Universidad Politécnica de Valencia – ITQ*

Gustavo Javier Chacón completed his Ph.D. in Chemistry from LUZ-IVIC (Venezuela) and UPS (France) in homogeneous and colloidal transition metal catalysts. From 2015 to 2023 acted as a postdoctoral researcher in the group of Prof. Jairton Dupont (Brazil) working on sustainable chemistry. Currently is a ComFuturo/MSCA researcher at ITQ in Valencia, leading the SUNAPPLIGHT project financed by the FGCSIC and CEPESA to develop hybrid materials for alternative energies.



Hakim Faraji *University of La Laguna*

Hakim Faraji holds a doctorate in Analytical Chemistry from Azad University and has been a faculty member there for several years. Since 2022, he has served as a Maria Zambrano Research Fellow at the University of La Laguna in Spain. His research experience extends to the Department of Neurochemistry at the University of Illinois at Urbana-Champaign, USA. Dr. Faraji specializes in interdisciplinary interfacial chemistry, focusing on bioanalytical and green analytical chemistry. His expertise covers the synthesis of environmentally friendly materials and techniques related to analytical sample pretreatment.



Ricardo Adolfo Medina Echavarría *University of Manizales*

Ricardo Adolfo Medina Echavarría is a physical engineer graduated in 2010 and professor at the University from Manizales since 2016, with experience in research in synthesis and characterization in semiconductor nanostructures with applications in spintronics and solar cells. Currently he is a PhD student in Physics Sciences from the National University of Colombia and Doctoral Candidate, with his thesis project aimed at making a solar cell prototype.



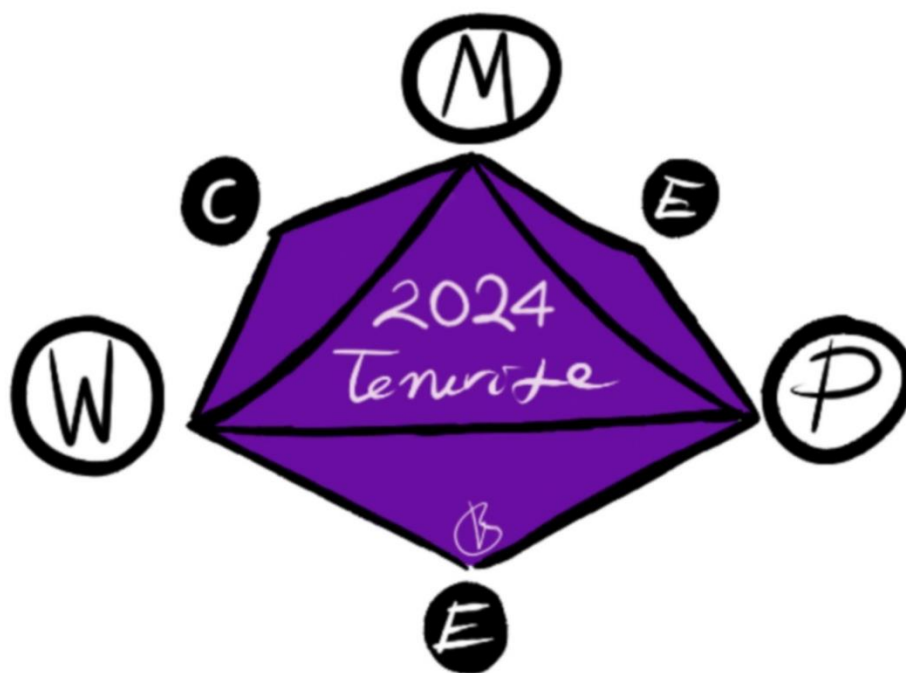
Yolanda Pérez Cortés *Universidad Rey Juan Carlos*

Since 2017, **Yolanda Pérez** is associate professor at Rey Juan Carlos University, and since 2020, she is senior assistant researcher in the group of Dr. Patricia Horcajada (Advanced Porous Materials Unit) at IMDEA Energy Institute (Excellence Center María de Maeztu). She is currently focused on the development of multifunctional materials for different social concerns: for performing chemical processes using clean energy and for environmental remediation. In this sense, Dr. Yolanda Pérez has participated in more than 20 research projects and published more than 50 scientific papers in high-impact international journals indexed in JCR.



Orhan Sisman *Alexander Dubček University of Trenčín*

Orhan Sisman completed his Ph.D. degree from the Sensor Laboratory at the University of Brescia, where he was supervised by Assoc. Prof. Dario Zappa and Prof. Elisabetta Comini. Currently, he is working as a postdoctoral researcher at the FunGlass Research Center, located at Alexander Dubcek University of Trenčín. His research interest lies in functional glass and glass ceramics designed for energy applications. He has actively participated in numerous EU-funded research projects.



**FLASH AND POSTER
COMMUNICATIONS OF THE
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Abraham Castilla Silvestre *University of La Laguna*

Abraham Castilla Silvestre is a PhD student in the Surface Science and Electrocatalysis Group at the University of La Laguna, under the guidance of Prof. Elena Pastor Tejera. Currently, he is immersed in the research of Direct Ammonia Fuel Cells as main topic of his doctoral thesis. His work involves investigating new materials to enhance the efficiency of ammonia oxidation reaction (AOR) and oxygen reduction reaction (ORR).

Maria Luisa Marín *Universidad Politécnica de Valencia – ITQ*

Maria Luisa Marín currently co-leads the Supported Photoactive Materials team (PAMA, <https://pama.itq.webs.upv.es/>) at the Institute of Chemical Technology (ITQ, UPV-CSIC). Current research topics are focused on the design, synthesis, and characterization of new heterogeneous photocatalysts for wastewater remediation, more sustainable chemical processes, and H₂ generation. Our interests range from understanding their performance to scaling them up for industrial applications.

Airán Ródenas Seguí *University of La Laguna*

Dr. Ródenas is a Ramón y Cajal Spanish fellow and professor at the Physics Department of Universidad de La Laguna. He graduated with a PhD in Physics at the Universidad Autónoma de Madrid in 2009 and has worked as senior researcher at Heriot Watt University (UK), Universitat Rovira i Virgili (Spain), and the Institute of Photonics and Nanotechnology (IFN) of the National Research Council (CNR) of Italy. He now leads the LeapLab group (Light-Matter interactions and Extreme Applications Photonics Lab) at the Physics Department of the Universidad de La Laguna (ULL).

Daniel Ballesteros Plata *University of Málaga*

Since 2015, **Dr. Daniel Ballesteros Plata** works in the Department of Inorganic Chemistry, Crystallography and Mineralogy at the University of Malaga, His research is focused on the synthesis of supported heterogeneous transition metal catalysts applied for the valorization of lignocellulosic biomass in chemical products (HDO reactions). Also, his research is focused on CO₂ capture and on catalytic valorization of CO₂ and N₂O to obtain chemical products of industrial interest such as propylene, dimethyl ether, and methanol.

Manuel Cruz Yusta *University of Córdoba*

Dr. Manuel Cruz Yusta is scientist with over 20 years of experience in research and development. He began his research career focusing on the energy sector, specifically developing small-sized lead-acid batteries that could be used as UPS. During his postdoctoral stage, he started working in the construction materials sector, specifically in the valorization of waste and its utilization as photocatalytic materials for the decontamination of NO_x gases. Currently, he remains active in both areas, contributing to the development of construction materials and new photocatalysts.

Laura Díaz Rodríguez *University of La Laguna*

Laura Díaz, a researcher in the "Heterogeneous Catalysis" group at the University of La Laguna, specializes in the synthesis, characterization, and study of the catalytic activity of porous materials to produce biofuels and the purification of water and oils. With two six-year research periods (2010-2016; 2017-2022), 25 publications, and over 30 participations in conferences, she has led two research projects and holds two patents and a utility model in the field of inventions.



Elisenda Pulido Melián *University of Las Palmas de Gran Canaria*

Elisenda Pulido Melián obtained her degree in Chemistry and Ph.D. in Environmental Engineering and Desalination at the University of Las Palmas de Gran Canaria. She is member of the Research Group Photocatalysis and Spectroscopy for Environmental Applications (FEAM) since 2005 and currently Associate Professor at the University of Las Palmas de Gran Canaria. Her activity is focused on photocatalysis (oxidation of VOC's and NO_x, water photosplitting, photoreforming and CO₂ photoreduction) and synthesis of new materials for this application.



Karina Rodríguez Espinosa *University of La Laguna*

Karina Elvira Rodríguez Espinoza, a researcher in the "Heterogeneous Catalysis" group at the University of La Laguna, has extensive experience in the synthesis, characterization and study of the catalytic activity of porous materials for industrial processes such as the production of biofuels. A six-year period of research, 19 publications and 39 presentations at conferences, participation in 10 research projects obtained in public calls on the subject of Catalysis, Biofuels and Energy Use of Waste.



Fernando Tadeo *University of La Laguna*

Fernando Tadeo is a Professor at the School of Industrial Engineering of the University of Valladolid, Spain, doing multidisciplinary research focused on applications in Process Control (In particular in Desalination) and in Renewable Energies (Wind, Solar and Osmotic Energies). He is co-author of around 90 papers in international journals, and 200 conference presentations.

María del Carmen Román Martínez *University of Alicante*



Maria del Carmen Roman Martinez is Professor of the Department of Inorganic Chemistry and researcher at the Materials Institute of the University of Alicante (IUMA). Her research activity focuses in the field of catalysis, dealing with the preparation and characterization of several types of catalysts, applied in fine chemistry synthesis, dry reforming of methane, hydrolytic hydrogenation of cellulose and biomass, and in photocatalytic reactions to eliminate pollutants in gas and liquid phases and to generate of hydrogen by photo-reforming of biomass derivatives. She has participated in more than 25 research projects (public and private) and has been director or codirector of 12 PhD theses.

Jorge Pasán *University of La Laguna*



Jorge Pasán is a Fundación La Caixa – Fundación CajaCanarias Senior Excellence Researcher at the Inorganic Chemistry area of the Chemistry department at University of La Laguna. He obtained the PhD in Physics in 2006 with research about molecular magnetism and crystallography. From 2014 on his interests had drifted towards the use of metal-organic frameworks on analytical chemistry. He has coauthored more than 135 articles and I have participated in more than 10 research projects.

Isabel Barroso Martín *University of Malaga*



Isabel Barroso Martín is a chemical engineer and PhD within the Doctorate Program “Chemistry and chemical technology, materials and technology” from University of Málaga. She has two master’s degrees in applied chemistry for materials characterization and secondary education. She is currently working as a postdoctoral researcher in the Inorganic chemistry, crystallography, and mineralogy department of the University of Málaga, under the supervision of Prof. Dr. Enrique Rodríguez Castellón and Prf. Dr. Antonia Infantes Molina.

Diego Allgaier Díaz *University of La Laguna*



Isabel Barroso Martín is a chemical engineer and PhD within the Doctorate Program “Chemistry and chemical technology, materials and technology” from University of Málaga. She has two master’s degrees in applied chemistry for materials characterization and secondary education. She is currently working as a postdoctoral researcher in the Inorganic chemistry, crystallography and mineralogy department of the University of Málaga, under the supervision of Prof. Dr. Enrique Rodríguez Castellón and Prf. Dr. Antonia Infantes Molina.

Santiago Daniel Cabrera González *University of La Laguna*



Santiago D. Cabrera-González is a first year PhD student in Chemistry and Chemical Engineering at the University of La Laguna (ULL) under the direction of Dr. María J. Trujillo Rodríguez. He is a member of the Materials for Chemical Analysis ULLL (MAT4LL) research group, where his research focuses on the synthesis and characterisation of new functional materials for their application in chemical analysis methodologies. His ORCID number is 0009- 0002-6271-9187

Stefan Delgado Barreto *University of La Laguna*



Stefan Delgado Barreto is graduate chemist with experience in physical chemistry and over 5 years of research. Currently, predoctoral researcher, with knowledge in synthesis and physicochemical characterization of 2D materials and electrochemical characterization. 2 months of international internship at the Institute of Materials Engineering of the University of Rzeszow. Extensive experience in conferences and scientific dissemination.



Marta González Barrios *Universidad Complutense de Madrid*

Marta González Barrios was graduated in Experimental Sciences from Rey Juan Carlos University in 2020, and was awarded the Extraordinary End of Degree Prize. Subsequently, she pursued the Master's program in Chemical Science and Technology at Complutense University of Madrid (UCM) during the academic year 2020/2021. In 2021, she commenced a position as a Research Assistant through the Youth Employment Program of the Community of Madrid in the Department of Inorganic Chemistry at UCM. Presently, she is a recipient of the Predoctoral Scholarship from the Community of Madrid within the same department.



Irina Guerra-Martín *University of La Laguna*

Irina Guerra-Martín is a graduate in Chemistry from the University of La Laguna. Currently, she is a PhD student in Chemistry and Chemical Engineering at the University of La Laguna, focusing on the study of inks for coatings and other microextraction devices. She has participated in a total of 3 national congresses and 3 international ones (being recognized at ITP2023 as one of the top 6 young poster presenters). Additionally, she has a scientific publication in a journal indexed in quartile 1 of the JCR.



Sara Lara Torres *University of La Laguna*

Sara Lara Torres, graduated in Environmental Sciences, is hired as a pre-doctoral fellow by the ACIISI at the ULL where she develops her doctoral thesis in the MAT4LL group. During its development she has participated in publications in JCR journals, international, national and regional research projects and numerous communications at national and international conferences.



Yaiza Martín García *University of La Laguna*

Yaiza Martín García is a doctoral student in the Molecular Nanoscience and Nanotechnology program. She is dedicated to the design, synthesis and characterization of new materials aimed at the elimination of emerging contaminants. She graduated in Physics and specialized in Nanoscience and Molecular Nanotechnology.



Stephanie J. Martínez *University of La Laguna*

Motivated and proactive electrochemist with +4 years of experience in laboratory research and analysis and +6 years of scientific dissemination. Experienced in using Raman and Infrared spectroscopy, electrochemical studies, and fuel cell measurements. Collaborated with other scientists on research projects and shared knowledge (J. Heyrovsky Institute of Physical Chemistry-Prague, 2018 and Consiglio Nazionale delle Ricerche (CNR)-Institute of chemistry of the organometallic compounds (ICCOM) Florence, 2022-2023).



Norberto Medina Rodríguez *University of La Laguna*

Graduated in Physics from the University of La Laguna, **Norberto Medina Rodríguez** holds a master's degree in molecular Nanoscience and Nanotechnology. Currently pursuing a Ph.D. in Nanoscience and Nanotechnology, his research focuses on exploring the use of multivariate metal-organic frameworks (MTV-MOFs) for the design and development of new microextraction devices.



Patricia I. Napolitano Tabares *University of La Laguna*

Patricia I. Napolitano Tabares is a predoctoral researcher at the University of La Laguna, where she is also pursuing her PhD in the Chemistry and Chemical Engineering program. She is under the guidance of Prof. Verónica Pino and Prof. Ana I. Jiménez Abizanda. Her research is primarily focused on the development of new materials and devices for sample preparation and analysis in the field of Analytical Chemistry.



Isaac Negrín Santamaría *University of La Laguna*

I finished my Chemistry Degree in 2020 at University of La Laguna, finishing my Chemistry as well master's degree in 2021 at the same university. In 2021 I started my PhD studies in Analytical Chemistry field, obtaining a FPI fellowship in 2022 from ACIISI agency. Since then, I have focused my research on the development of miniaturized devices based on metal-organic frameworks for bioanalytical applications and environmental monitoring.



Jose Aythami Pérez Remedios *University of La Laguna*

Jose Aythami Pérez earned a degree in industrial chemical engineering and a master's in renewable energies from the University of La Laguna. Currently, he is pursuing a Ph.D. in chemistry and chemical engineering at the same university, supported by the Santander-University of La Laguna predoctoral fellowship. His doctoral research is focused on investigating the energy potential of animal by-products not intended for human consumption (ABP), exploring their transformation into biofuels such as biogas, biomethane, dimethyl ether (bioDME) and hydrogen. Currently, he is member of the Heterogeneous Catalysis Research Group at the University of La Laguna.



Maja Ostojic *Universidad Complutense de Madrid*

Maja Ostojic is research assistant at the department of Inorganic Chemistry, Faculty of Chemistry, UCM, Madrid, Spain (Dec 2023 – present), Chemistry Intern at the Institute CBMN, Bordeaux, France (Oct 2022 – July 2023), research assistant at the Institute of Chemistry, Technology and Metallurgy (Feb 2022 – June 2022).

Education: MSc in Analytical Chemistry of Drugs and Natural Products (2022-2023, Bordeaux, France), BSc in Biochemistry (2018-2022, Belgrade, Serbia)



Yapci Remedios Diaz *University of La Laguna*

Yapci Remedios is a graduated chemist with experience in the area of physical chemistry for four years to date. Predoctoral researcher with knowledge in physicochemical and electrochemical characterization of two-dimensional materials, especially in MXenes and dichalcogenides. Experience in scientific dissemination and organization of I+D activities as an organizing committee. Participation in numerous national and international congresses.



Jennifer Rodríguez González *University of La Laguna*

Jennifer Rodríguez is graduated in Chemistry and with a Master's Degree in Chemistry in the specialty of Environmental, Agri-Food and Materials Chemistry. In addition, through the Cepsa Foundation Chair in Ecological Transition and Innovation, she was awarded 1st prize for both the Final Degree Project and the Master's Final Project. She is currently working in the General Research Support Service of the University of La Laguna in the Infrared Spectroscopy Service.



Alejandro Rodríguez González *University of La Laguna*

Alejandro Rodríguez is a PhD student in Chemistry and Chemical Engineering at the University of La Laguna. He is a member of the Materials for Chemical Analysis Group (MAT4LL), where his research focuses on the development, synthesis and characterization of new, smart, sustainable, selective, and efficient materials for their implementation in chemical analysis methodologies.



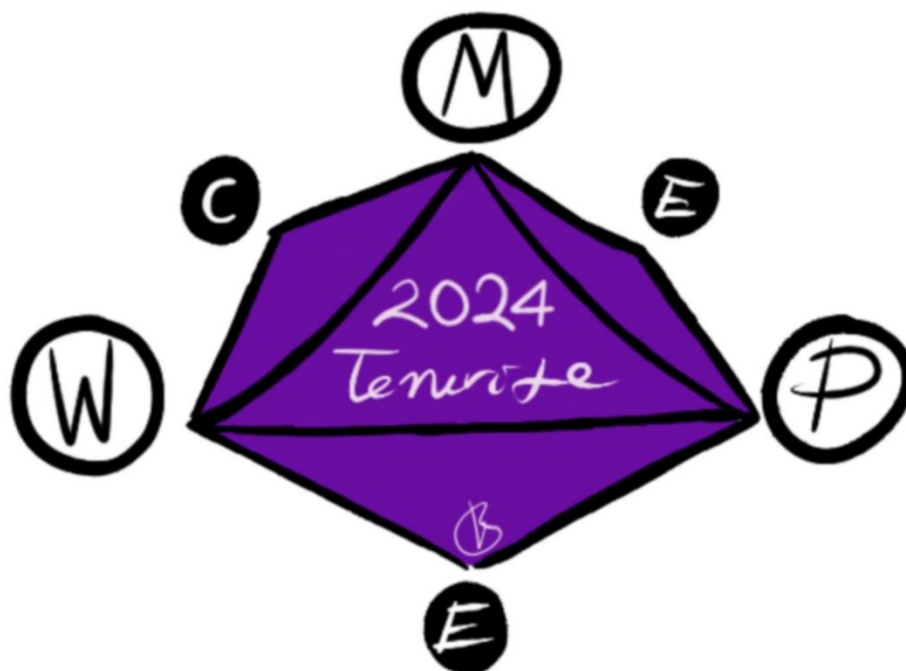
Agoney González Cabrera *University of La Laguna*

Agoney González is a chemistry graduate from the University of La Laguna. He has a presentation at the XV Chemistry Section Student Congress titled 'Visible Light Diffraction, Prelude to the Double-Slit Experiment,' which received an award for being one of the best presentations at the event. Currently, he is pursuing a master's in chemistry at University of La Laguna, and his thesis focuses on the study of heterogeneous catalysis for conducting tandem reactions.

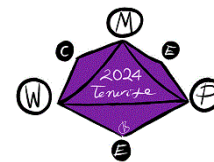


Noura AFLAK *Cadi Ayyad University*

Noura AFLAK holds a PhD in sustainable catalysis and organic chemistry from Cadi Ayyad University. She also holds at the same university a master's degree in biopolymers and a bachelor's degree in industrial chemistry. Her research focuses on the development of green homogeneous and heterogeneous catalysts for synthesizing organic compounds.



**ABSTRACTS OF THE
“II WORKSHOP ON MATERIALS FOR
PHOTOCATALYSIS, ENERGY, AND
CLEAN ENVIRONMENT”**



Advanced materials for Li and Na-ion battery technologies: Effect on the energy transition

N. Nieto, J. Rodríguez, E. Redondo, V. Palomares, E. Goikolea, I. Ruiz de Larramendi,
L- Lezama and T. Rojo

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Achieving net-zero emissions requires a radical transformation in the way we supply, transform and use energy. Battery energy storage systems (BESS) with high electrochemical performance are one of the prominent alternatives towards reducing greenhouse gas (GHG) emission and decarbonization. The battery technology is critical for enabling renewable yet intermittent sources of energy such as solar and wind. In recent years, numerous new battery technologies have been achieved and showed great potential for mobility and stationary energy storage applications. The increasing interest in energy storage for the grid can be attributed to multiple factors, including the capital costs of managing peak demands, the investments needed for grid reliability, and the integration of renewable energy sources.

Among the existing energy storage technologies, lithium-ion batteries (LIBs) have unmatched energy density and versatility and are the most adequate to be used in portable market and electrical vehicles. However, because LIB raw material deposits are unevenly distributed and prone to price fluctuations, these large-scale applications have put unprecedented pressure on the LIB value chain, resulting in the need for alternative energy storage chemistries. In this context, Sodium-ion batteries (SIBs) are under continuous progress and they will be a critical technology in the coming post-lithium era, as they provide a low-cost energy storage solution from earth abundant resources. Developing advanced materials for both systems is the key to clean energy, and clean mobility technologies in the future and (due to industry 4.0) will soon account for 80% of the technology manufacturing cost.

In this talk, we will analyze recent progress, exiting challenges and the overall requirements with key parameters for Li and Na-ion battery technologies for practical applications.

Modifying hematite to enhance photoelectrocatalytic activity for water oxidation

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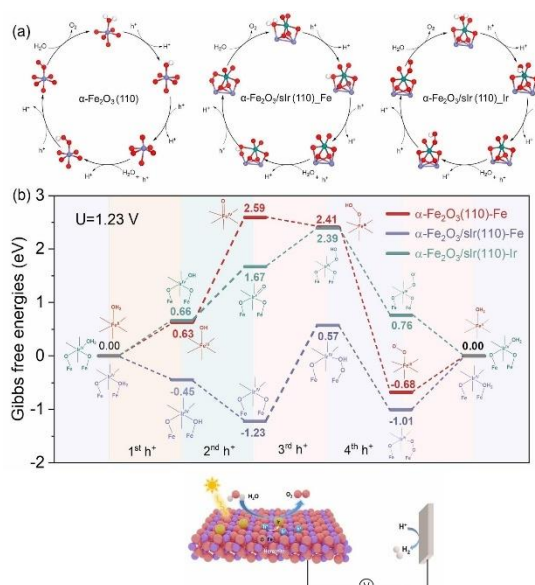


Figure 1. DFT calculations on hematite/sir system [2]

Hematite is a promising candidate as photoanode for solar-driven water splitting. However, the interfacial charge transfer and recombination greatly limits its activity for photoelectrochemical water splitting. Here I will present two approaches developed in our group to promote catalytic activity of hematite: (1) We developed a novel carbon underlayer from low-cost and biomass-derived carbon dots through a facile hydrothermal process, introduced between the FTO substrate and hematite, leading to a remarkable enhancement of the photocurrent density amid a significant increase in charge transfer rate and lifetime of photogenerated electrons [1]. 2) Single-atom catalysts (SACs) are efficient cocatalysts to boost photoelectrochemical performance. They feature high atom utilization, remarkable activity, and distinct active sites. However, the specific

role of SACs on hematite photoanodes is not fully understood yet. By combining spectroscopic techniques and computing simulations (Figure 1), we demonstrate that single-atom iridium (slr) catalysts on hematite ($\alpha\text{-Fe}_2\text{O}_3/\text{slr}$) photoanodes act as a true catalyst by trapping holes from hematite and providing active sites for the water oxidation reaction [2]

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Applying photocatalysis to the regeneration of saturated granular activated carbon used in water treatment: a pilot scale study

Adnane¹, N. El-Ouahedy¹, K. Maiga¹, Y. Ballesteros², R. Torio², C.O. Ania¹

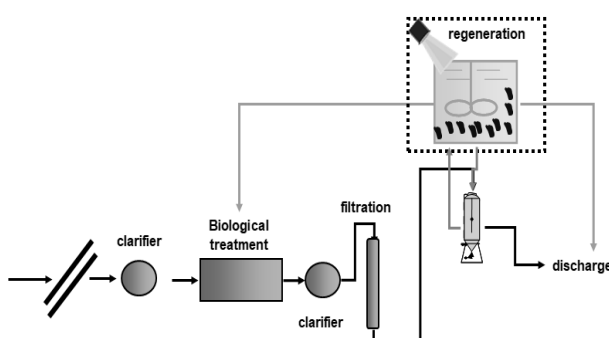
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Current challenges in wastewater treatment are linked to the need for developing effective solutions to face emerging pollutants, capable of removing the pollution while assuring a feasible economic upgrade of existing plants, as new investments are often limited by the economic constraints of different countries. Despite adsorption using activated carbons is a mature technology for the removal of emerging pollutants, the cost associated to the regeneration of the spent carbon columns (energy consumption, transportation) still represents a major limitation for further implementation [1]. Hence, the reactivation of saturated activated carbons is a crucial aspect in the upgrading and restructuring of existing water and wastewater treatment plants.

On the other hand, our pioneering studies have pointed out the ability of nanoporous carbons to generate radical oxygen species upon illumination, showing that nanopore confinement is critical for boosting charge transfer and inducing the photooxidative degradation of pollutants adsorbed in the porosity of carbon adsorbents [2,3]. This work describes the photocatalytic regeneration of spent activated carbons upon UV exposure in aqueous environments. Irradiation of the spent

carbon resulted in a gradual regeneration, which efficiency depended on the saturation state of the carbon and the illumination time. A fraction of the pollutants retained in the porosity of the carbon may be released into the solution upon illumination of the carbon particles, being subsequently photodegraded. Furthermore, data of a case study on spent activated carbons from a wastewater treatment plant equipped with activated sludge technology and granular activated carbon in Almendralejo (Spain) will be presented and discussed in terms of the quality of the reactivated carbon for further reutilization at the WWTP, and the quality of the effluent generated upon the treatment [4].

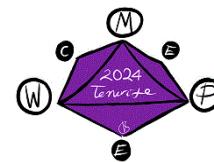


Acknowledgements

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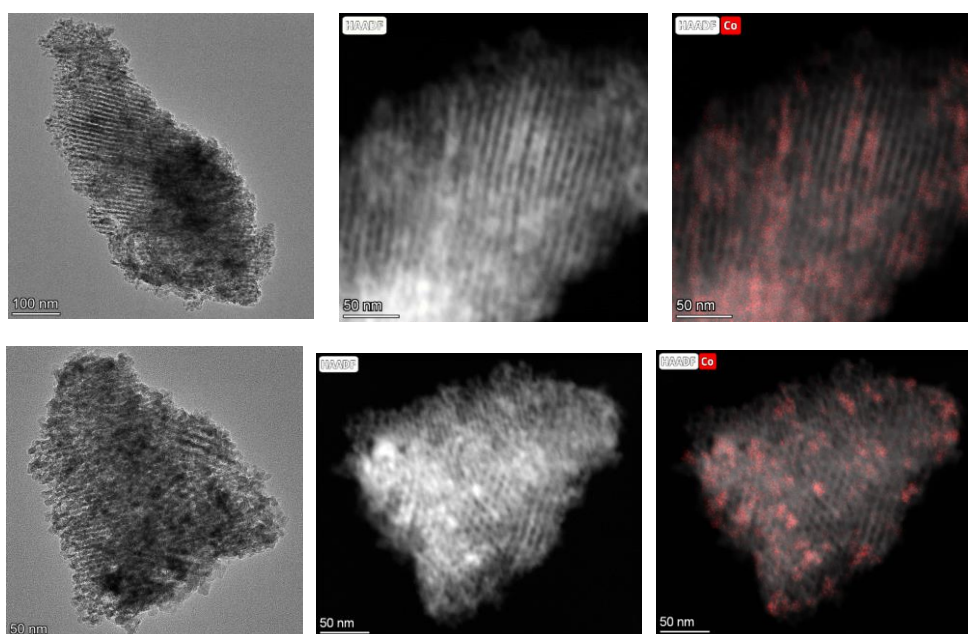
Cobalt-based mesoporous TiO₂ catalyst for Fischer-Tropsch reaction

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In this contribution, we show how a Cobalt supported on mesostructured TiO₂ catalysts prepared by a wet-impregnation method shows a better catalytic performance than a conventional Co/TiO₂-P25 system. TEM images show Co nanoparticles well distributed along the mesopore channels of TiO₂. Although the reduction pretreatment and reaction, induce a drastic structural change of mesopores, the high catalytic performance is maintained.

We conclude that the confinement of Co particles 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.



Acknowledgments

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Carbon-based nanostructured composite (piezo)photocatalysts: energy and organic redox synthesis applications”

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This work is a report of recently selected experiments on (piezo)photocatalysts fabricated by (among others) ultrasound-based techniques, and their application in photocatalytic selective oxidation of organics (e.g. benzyl alcohol, BnOH, as a model bio-oil-based compound), and water decontamination in the frame of the concept of lignin valorization (Figure 1A), and the proof of concept of intensifying a flow photocatalytic oxidation process by sonication (Figure 1B). The lecture will be divided into the following case studies:

1. Preparation and characterization of highly functional biochar-based support for TiO₂: sustainable gaseous selective oxidative esterification of methanol to methyl formate and phenol degradation in water [1].
2. Titania/Chitosan-Lignin nanocomposite as an efficient photocatalyst for the selective oxidation of benzyl alcohol under UV and visible light [2].
3. Investigation of the Sonocatalytic Activity of Porous Heteroatom-Doped Carbonaceous Materials for the Selective Oxidation of 4-hydroxy-3,5-dimethoxybenzyl Alcohol.

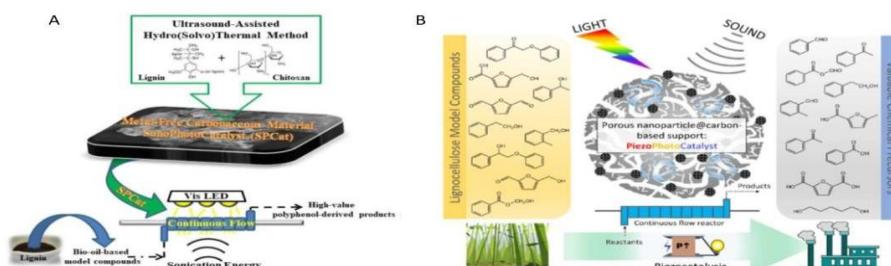


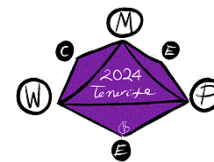
Figure 1. **A.** Carbo(piezo)photocatalysts based on lignin and chitosan, **B.** Porous carbon-based materials for lignin valorisation.

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Acknowledgments

The National Science Centre (NCN) in Poland within research project OPUS 20 No. 2020/39/B/ST5/00076 <https://photocatalysis.org/projects/nanoengineering-of-multicomponent-metal-free-carbonaceous-materials-for-bio-oil>



Thermal assisted photocatalysis for energy applications: H₂ production and CO₂ valorisation

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It raised a common consensus that all joint efforts shall be oriented to limit the increase in the global average temperature to less than 2°C above preindustrial levels. In order to reach this objective, the decrease of CO₂ emissions is compulsory. So, changing our energy vectors to renewables and developing a low carbon economy might be considered as the main milestones. The use of different energy sources and softer conditions for the catalysts has been recently suggested as a novel approach pursuing the improving efficiency of the catalytic process. Therefore, combined processes, photo- and thermal-, with specific synergetic effect is nowadays a novel unexplored roadway that could help this attractive technology to become feasible for large scale energy production. Thus, the illumination of the catalyst by light will increase the local temperature via the photothermal effect, which then drives the reported energy related reactions.

In this way, thermo-photocatalysis emerges as an enormously interesting new approach that can be especially decisive for both H₂ production and CO₂ valorisation reactions. In recent years, the concept of the '*thermophoto*' effect has emerged (in some cases the term '*photo-thermal*' has been used), in which the need has arisen to develop a superior catalytic system that incorporates the positive aspects of photocatalysis with those of traditional thermal catalysis in order to have greater catalytic activity and applicability in the framework of renewable solar energy.

We are presenting two interesting examples in which thermo-phocatalysis provides new insights with traditional photocatalysis, and also would be considered an interesting alternative to conventional thermal catalysis (Figure 1).

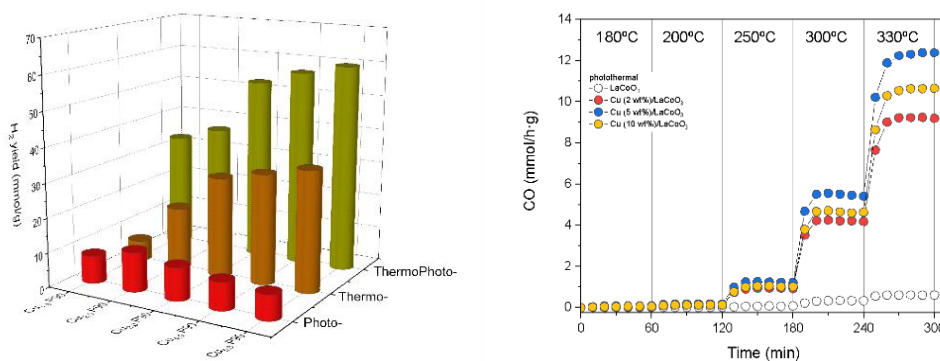


Figure 1. H₂ yield from methanol reforming (left); evolution of CO with temperature during rWGS (right) by thermo-photocatalysis.

Alkaline CO reduction at modified Cu single crystals - Chasing the selective formation of ethanol

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Carbon dioxide capture and conversion into valuable chemicals is a key step in the development of new eco-friendly industrial processes. Currently, the reduction of CO₂ to CO is well developed, but further reactivity into specific products is still challenging. In this sense, the electrochemical CO reduction reaction (CORR) has been proposed as a suitable method for the generation of both C1 (CH₄, CH₃OH, etc.) and C2 (CH₃CH₂OH, C₂H₄, etc.) products. Cu-based catalysts are well studied materials for this reaction, presenting high catalytic activity and faradaic efficiency [1]. However, they present a lack of selectivity and produce a variety of C1 and C2 products during their performance.

In this work, Cu(hkl) surfaces have been modified with Co(OH)₂ [2] and tested towards CORR in alkaline medium. The catalytic performance has been studied using *in-situ* Differential Electrochemical Mass Spectrometry (DEMS) and *ex-situ* Nuclear Magnetic Resonance (NMR) of the electrolyte after polarization. Further characterization of the surface under reaction conditions have been obtained by means of *in-situ* Electrochemical Scanning Tunneling Microscopy (EC-STM) and *in-situ* Raman Spectroscopy.

Results (Figure 1A) show a remarkable electrochemical performance of the modified single crystal towards the specific formation of EtOH during alkaline CORR. Both DEMS and NMR experiments prove the exclusive formation of EtOH and H₂ during polarization of the Co(OH)₂-modified Cu surfaces with a faradaic efficiency towards ethanol of around 60 %.

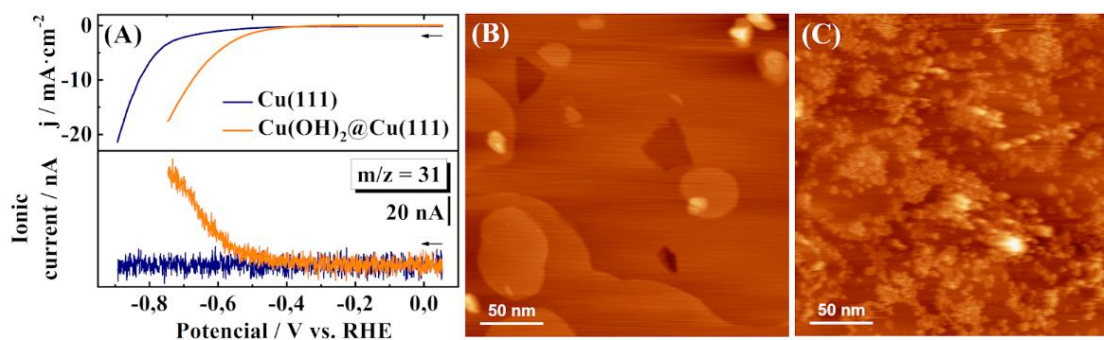


Figure 1. (A) DEMS experiments recorded for the CORR on pristine Cu(111) and Co(OH)₂@Cu(111) catalysts in 0.1 M NaOH at 1 mV·s⁻¹. Top panel shows the current density and bottom panel shows the m/z = 31 (CH₃O⁺) signal during polarization. EC-STM image of (B) the pristine Cu(111) and (C) the Co(OH)₂@Cu(111) surfaces.

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Photocatalysis: Quantitative analysis of photo and thermo-photo reactions

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The efficiency of photon-based single and dual (thermo-photo) chemical processes is analysed on quantitative basis using the different families of physico-chemical observables commonly utilized in the literature. For both types of processes, the chemical, photonic and energy balances will be analysed in terms of the adequate mathematical formulation of the corresponding physicochemical parameters as well as their physicochemical interpretation. Such an analysis will be presented using most typical single and composite catalytic materials. [1-3].

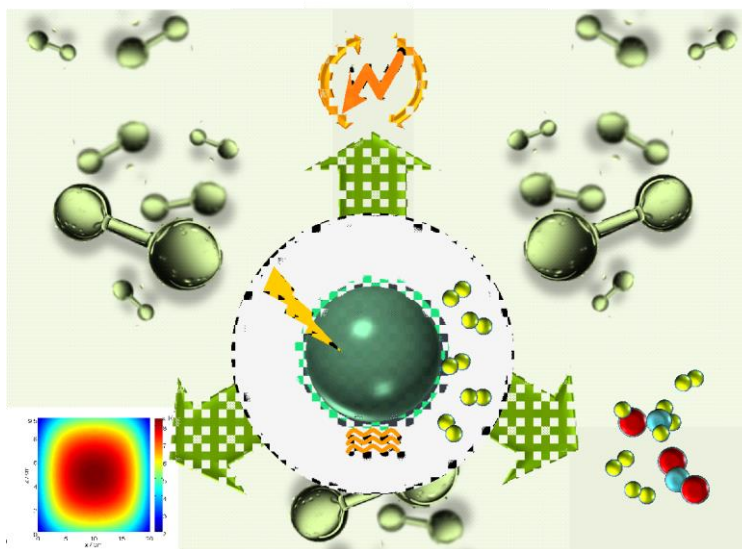
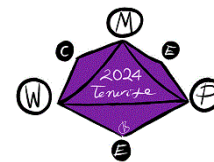


Figure 1. Representation of the energy source nature/characteristics and main physicochemical affecting catalytic performance.

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High-throughput screening of thermoelectric materials by machine learning

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Approximately, 70 percent of energy produced by humans is wasted as heat, hence, improving the efficiency of the grid is as important as using environmentally friendly energy sources. Thermoelectricity stands out as one of the best solutions to recycle that heat, producing electricity. The discovery or optimization of more efficient and less expensive thermoelectric materials cannot be seen as an easy task. During the last decades, significant resources have been dedicated to the improvement of the efficiency of these materials, measured by its figure of merit, ZT . The importance of computational material science in the discovery of new thermoelectric materials has run in parallel to the development of new frameworks and methodologies to compute the electron and thermal transport properties linked to ZT . A large set of methods, packages and frameworks have been developed during the last twenty years to predict the aforementioned properties [1]. The main disadvantage underneath all these options stems from the accuracy-computational cost trade-off. In the last years, new approaches have been developed to reduce the computational cost or the need of experimental data without compromising the accuracy of the results. The use of machine learning techniques in the calculation of interatomic force constants has drastically reduced one or two orders of magnitude the computational cost of predicting the lattice thermal conductivity of solids using the Boltzmann transport equation [2]. On the other hand, new efficient methods have been reported for calculating carrier scattering rates of semiconductors and insulators from first principles without any external parameter [3]. To the best of our knowledge, we combine these new strategies to compute ZT for first time. This approach does not only guarantee accurate values for ZT but also reduces the cost, giving the opportunity of studying larger sets of materials to understand the physical and chemical factors that govern thermoelectricity. In this work, the whole family of skutterudites MX_3 ($M = \text{Co, Rh, Ir}$; $X = \text{P, As, Sb}$), as well as selected chalcogenides and oxychalcogenides with high potential applications in thermoelectrics, are explored.

Acknowledgments

Funded by Spanish MICIN/AEI/10.13039/501100011033 and by “EU Next Generation EU/PRTR” (grants PID2022-138063OB-I00 and TED2021-130874B-I00).

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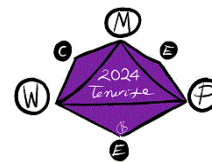


Photo and thermo-photo production of hydrogen from bio-molecules

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Hydrogen production from bio-alcohols is explored using photo and thermo-photo catalysis. In this talk we will focus on results using noble and non-noble metal TiO₂-based catalysts (see Figure 1 as a schematic representation of a typical system) as well as the interpretation of the activity through new activity-structure relationships established through the combination of mechanism-kinetic and operando spectroscopic studies. Several examples containing mono and bimetallic co-catalysts as well complex and mixed oxides will be presented [1-4].

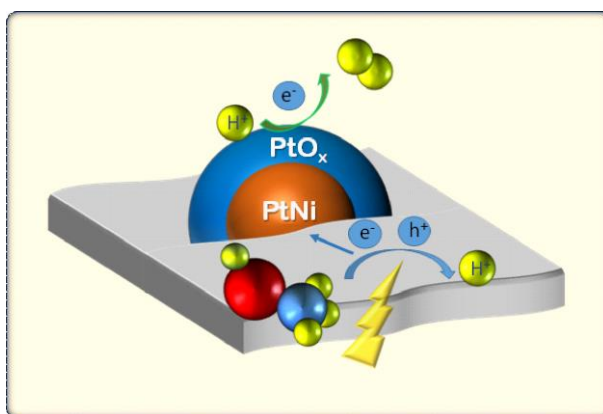
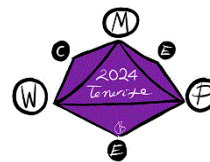


Figure 1. Schematic representation of hydrogen photo-production from methanol using a composite metal-oxide catalyst.

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Customizing inorganic nanomaterials synthesis for environmental remediation

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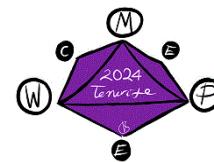
The synthesis of inorganic nanomaterials has been revolutionized by the impact of chemical approaches that allow us to precisely tune the size, composition, morphology, and microstructure of the solid-state materials produced. In particular, tuning the morphological features of a material has emerged as an important strategy to improve its catalytic/photocatalytic performance, and there has been extensive research to develop highly active ceramic systems rationally designed with a controlled shape and an ordered porosity at the nano/microscale for environmental applications.

This talk will focus on the importance of tuning the morphological features of a catalyst as a strategy to improve its photoactivity, focusing on how rationally designing inorganic nanomaterials can lead to physico-chemical and optical properties able to enhance the performance in industrially and environmentally important processes.

The talk will discuss some applications that can be addressed by multi-component systems highlighting their structure-reactivity relationship. Photodegradation of selected drugs will be presented as successful case history [1, 2].

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Noble metal-free catalysts for electrolyzers and fuel cells

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Hydrogen is considered an energy vector for the transition towards a future based on the use of renewable energy. In this context, electrolyzers (EL) allow to obtain H₂ of high purity, which would be a great advantage when used in low-temperature fuel cells (PEMFC). However, the development of these systems and their entry into the market are conditioned, in part, by the use of noble metal catalysts (platinum group metals, PGMs). This communication presents the latest results of our research group in the preparation of materials free of noble metals with high activity for the reactions on the electrodes of these devices.

In the field of EL, transition metal carbides appear as an alternative to PGMs developing good catalytic activity towards the electrochemical generation of hydrogen. In the search for cheaper materials, the use of ionic liquids that improve the mechanical resistance and electrical conductivity of the resulting composite materials has also been proposed. The study of the hydrogen evolution reaction by means of differential electrochemical mass spectrometry (DEMS) has allowed us to explore the mechanistic aspects of this process.

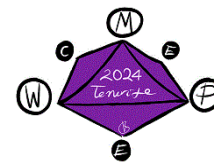
On the other hand, graphene materials (MGs) have recently shown their potential as a support for electrocatalysts, with important activities, even similar, to those of materials based on platinum and other noble metals. The doping of MGs also appears as an appropriate method to modify and control the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

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Layered cathode architectures deposited by spray pyrolysis for optimised solid oxide cells

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The need for a self-sustainable energy sector, with emphasis on green-energy development is expounded by the European Green Deal, which has set the goal of zero greenhouse-gas emissions for 2050 [1]. In this context, hydrogen is a viable alternative to fossil fuels, converting chemical energy to electrical energy in fuel cells with high efficiency and zero emissions. Nevertheless, green-hydrogen production requires significant development of zero-emission technologies such as electrolysis cells. Solid oxide cells (SOCs) are good candidates to produce green hydrogen from renewable energy in low-demand periods and convert it to electrical energy in highly demanding periods. The high operating temperature of SOC leads to improved efficiencies but decreases durability [2]. Reducing the working temperature to the intermediate range (500 – 800 °C) requires innovative solutions to enhance the electrochemical performance of the components, mainly of the air electrode, which suffers from high polarisation as temperature decreases. Air electrodes with layered architectures may be used to optimise microstructure and interfacial properties to tailor the electrochemical properties of the components.

In this work, spray pyrolysis is employed to produce highly efficient air electrodes at low processing temperature, resulting in optimised microstructures with small grain sizes and concomitantly high electrochemical active area. The technique is suitable for benefitting the production of active interlayers with tuned mixed transport properties, or multilayers, with adjusted electrochemical behaviour and thermal features. The implemented methodologies produced electrochemical cells with improved performances and stability, with high potential for application in scalable devices.

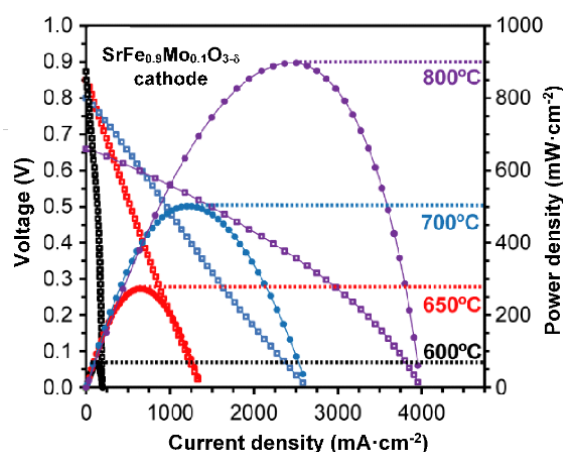
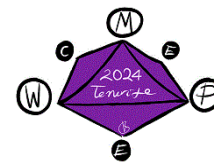


Figure 1. Voltage and power-density curves as functions of current density for a ceria-based single solid oxide fuel cell with a $\text{SrFe}_{0.9}\text{Mo}_{0.1}\text{O}_{3-\delta}$ cathode prepared by spray pyrolysis.

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Nickel hexacyanoferrate nanocubes as highly performing catalyst for solar-light-driven photodegradation of metronidazole

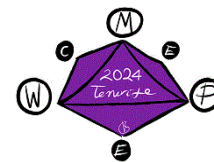
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Environmental pollution, particularly that one regarding the presence of drugs in wastewater, has dramatically increased and is also posing serious issues for the public health. In recent years, the interest of the scientific community has been devoted to address these issues by developing new engineered materials. Here we describe our recent findings concerning the photocatalytic activity of Ni-hexacyanoferrate (Ni-HCF) nanocubes, which has been investigated in the photodegradation of aqueous solutions of metronidazole (MDZ) under simulated solar light. Ni-HCF showed very promising results leading to ~95% yield for the MDZ degradation after 6 hours. The remarkable performance can be attributed to a higher ability in separating the charge carriers and to a lower charge transfer resistance, as demonstrated by electrochemical measurements. These achievements highlight the possibility to combine the performance of an earth-abundant catalysts with a renewable energy source for environmental remediation, meeting the requirements of a sustainable development.



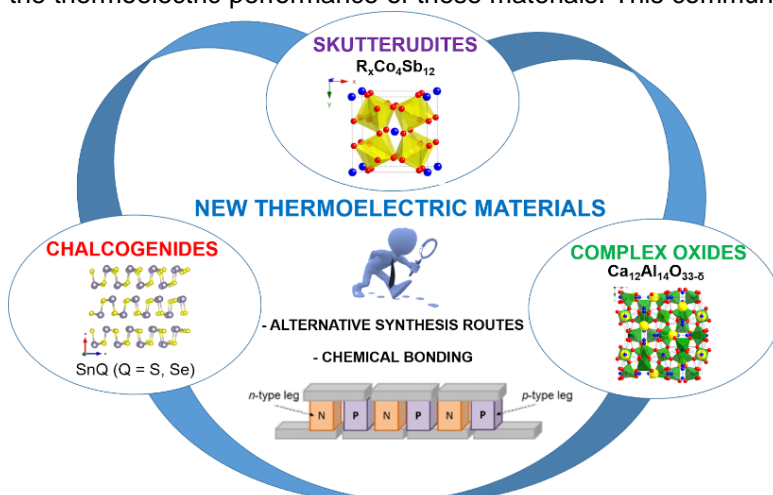
Harvesting power from waste heat: Unveiling the potential of thermoelectric materials for clean energy generation

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The urgent need for a green energy transition has reignited interest in thermoelectric (TE) materials as crucial components in sustainable technologies. TE devices, capable of converting heat energy into electricity, present an opportunity to harness waste heat and improve energy generation efficiency. Given that around 60% of global energy is lost as heat, even recovering a modest 10% could surpass the combined output of current renewables. The efficiency of TE materials hinges on optimizing three interconnected properties of semiconducting materials: the Seebeck coefficient (S), electrical conductivity (σ), and thermal conductivity (κ). These properties collectively determine the figure of merit ($zT = S^2\sigma T/\kappa$), a key indicator of thermoelectric performance. While current commercially available materials have a figure of merit (zT) near unity, they primarily consist of toxic, scarce, or expensive elements (Bi_2Te_3 , Sb_2Te_3 , PbTe , SiGe). [1, 2]

In recent years, the development of new non-molecular inorganic materials and the exploration of novel strategies to optimize TE parameters, such as nanostructuring, doping, or controlling microstructure through alternative synthesis methods, have led to significant advancements in the thermoelectric performance of these materials. This communication will specifically focus on



the possibilities offered by material families, such as metallic chalcogenides, skutterudites, or complex oxides, with particular attention to the significance of the chemical bonding in them [3, 4]. In most cases, the proposed materials have been synthesized using "Rapid Chemistry" methods (mechanical milling, microwave-assisted synthesis, arc-melting, sol-

gel), and the relationship between their processing, structure, and properties has been investigated.

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2D/2D NiTi-LDH/BiOBr photocatalyst with extraordinary NO_x removal under visible light

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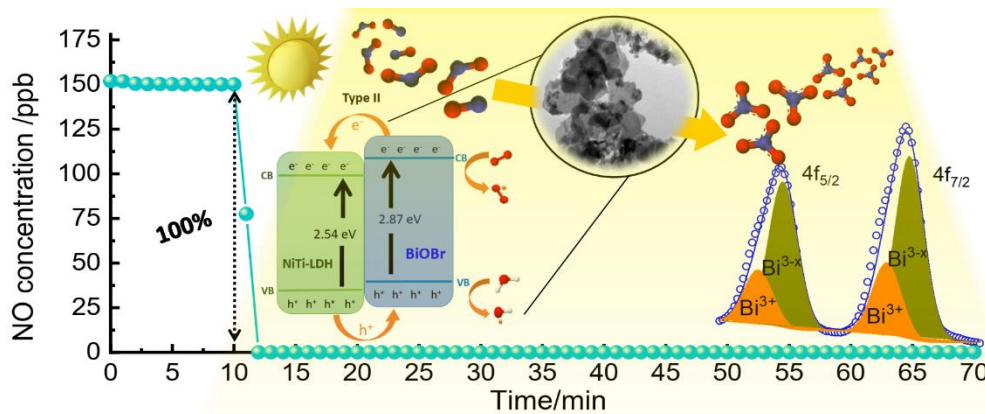
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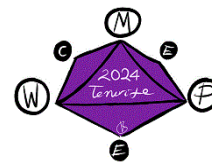
Many current studies are focused on the development of 2D/2D nanosystems based on non-traditional semiconductors as efficient visible light-active photocatalysts, due to their interesting structural and optical properties [1]. Thus, the charge-separation in heterostructures can be enhanced by boosting the interfacial contact [2]. In this work, robust 2D/2D NiTi/BiOBr composites have been prepared by incorporating a 2D layered BiOBr into NiTi-layered double hydroxides (LDH) for the subsequent study of their photocatalytic action in the control of NO_x pollution. The successful formation of a type-II heterojunction between both semiconductors has been confirmed by several characterization techniques (including XPS, NMR and electrochemical studies), indicating an intimate contact interface that helps enhance the visible light photocatalytic performance of NiTi-LDH. In particular, the NiTi-LDH/BiOBr-0.6 heterojunction, with a more efficient separation of photoinduced carriers, showed exceptional NO removal efficiency under visible light and remarkable robustness for the recycling process.



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Modification of nanostructured materials with natural dye sensitizers: applications in energy production and water electroremediation

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Industrialisation and energy consume have brought as consequence the contamination of water sources with compounds such as phenols, generating environmental and public health problems. Thus, search of alternatives to remediate contaminated water sources is mandatory to guarantee the access to potable water. Photocatalytic water splitting of phenol-containing water arises as an alternative to eliminate this substance through its oxidation, whereas green hydrogen is obtained by H^+ or OH^- reduction [1]. To perform this process, anatase phase- TiO_2 is commonly employed, but its high band gap (3.2 eV) forces the use of UV radiation to promote the water splitting [2]. Dye sensitizers adsorbed on anatase are a suitable alternative to reduce this band gap and promote the electron transfers in the presence of visible light and thus, with low energy [3].

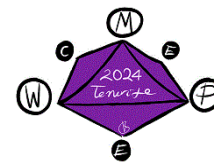
In this work, the performance of photocatalysts based on anatase phase- TiO_2 nanotubes and MXenes modified with dye sensitizers containing a high content of carotene, betalains and anthocyanins towards both, phenols oxidation and hydrogen reduction reactions, was established. The materials were physicochemically characterised by XRD, SEM-EDX, Raman spectroscopy, IR spectroscopy and diffuse reflectance spectroscopy. Moreover, linear sweep voltammetry, cyclic voltammetry and chronoamperometry were applied to verify their performance as catalysts for the mentioned reactions. MXenes in the presence of white light have promoted a shift in the onset potential associated to the hydrogen evolution reaction, meaning a low energy to address this reaction, and suggesting the suitability of these materials as cathodes for photoelectrolysers.

Acknowledgements

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Investigation of nano- and micro-photocatalytic systems *via* scanning electrochemical probe microscopy

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The generation of hydrogen (H₂) fuel via light-driven water splitting has attracted considerable interest over the last decades, due to its potential to contribute to the rising global energy demand and provide a solution to sustainable energy supply concerns. Given the complexity of developing molecular systems for H₂ production, it is crucial to comprehend the mechanisms that govern the solar-to-hydrogen conversion process and the stability of the photoactive systems [1]. The understanding of these systems encompasses the analysis of a variety of properties, such as photocatalytic activity, performance losses, and time-dependent degradation.

To this end, the co-deposition of microspotted arrays of photosensitizer (PS) and catalyst (CAT) opens the route for fast *in-situ* screening experiments to understand the photocatalytic performance and the degradation processes of different ratios of PS/CAT systems [2]. Scanning electrochemical probe microscopy techniques, such as scanning electrochemical cell microscopy (SECCM) [3] and scanning electrochemical microscopy (SECM) [4], using micro- and nanosized electrochemical probes allow local surface modification and provide (electro)analytical information on reaction dynamics [5] e.g., in situ quantification of light-driven hydrogen evolution rates.

In this contribution, light-driven molecular nano- and micro-systems consisting of cobaloxime-based catalysts and ruthenium polypyridyl-based photosensitizers will be presented. In particular, the *in-situ* and *operando* investigation of microarrays of co-deposited PS-CAT systems obtained *via* SECCM will be discussed with respect to the photocatalytic activity (H₂ evolution kinetics) and degradation processes using SECM, atomic force microscopy (AFM), and X-ray diffraction spectroscopy (XDS).

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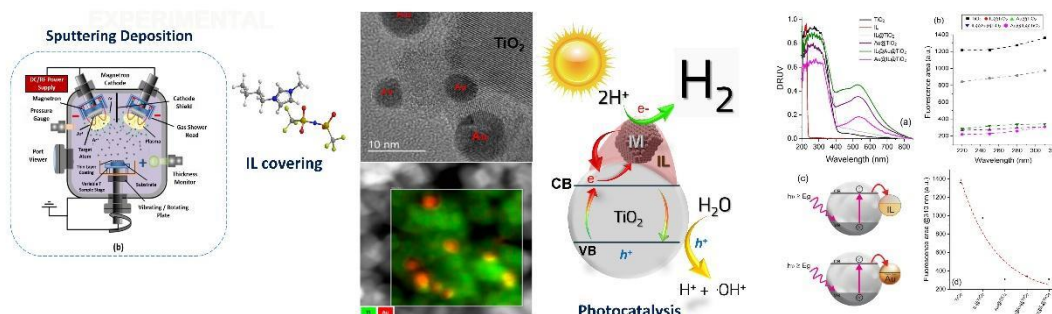
Advancing hydrogen production: Exploring alcohol photo reforming with hybrid gold based catalysts generated through physical enrichment

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The production of green hydrogen is a current area of research that seeks sustainable solutions for generating a clean and versatile fuel.[1] Metal Nanoparticles (MNPs) can perform numerous challenging chemical reactions with outstanding performance and specificity. In photocatalysis, MNPs with plasmon properties are one of the most employed due to their capacity of sensitizing semiconductor surface facilitating electron trapping and efficient charge separation.[2,3] In such devices, the visible light absorption of plasmonic allows the injection of their photoactivated electrons into the semiconductor conduction band, creating a charge separation that facilitates the Red-Ox process.[4] In hydrogen evolution reactions, these systems favour processes like Water Splitting Reaction (WSR). The magnetron sputtering offers exciting new opportunities for manufacturing supported MNPs since it usually generates highly active clean surfaces without chemical stabilizers and/or solvents.[5-7] Moreover, employing ionic liquid is an encouraging method for influencing the physicochemical characteristics of semiconductors via modulation of superficial electronic properties. [4,8] In this work, we present the preliminary results on the superior performance of IL@Au@TiO₂ type hybrid systems as promising systems for Hydrogen Evolution Reactions (HER) via photocatalytic WSR and Methanol Photo Reforming (MPR).



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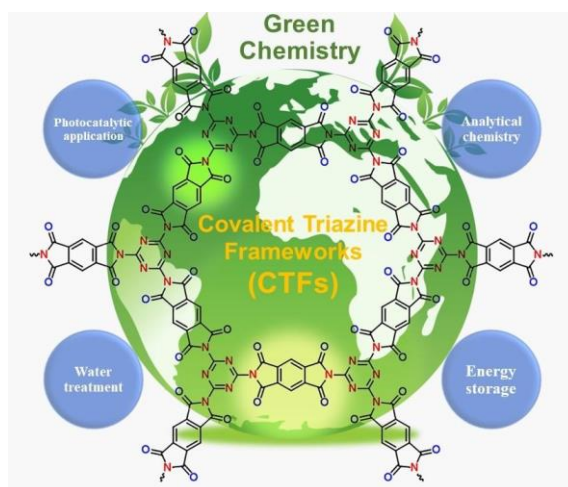
Covalent triazine frameworks for photocatalytic applications: challenges and new opportunities

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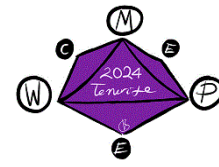
Covalent Triazine Frameworks (CTFs) have garnered considerable attention due to their distinctive structural characteristics, including a nitrogen-rich composition, fully conjugated framework, chemical stability, customizable pore size, expansive surface area, and exceptional porosity [1]. These inherent properties render CTFs highly appealing for a wide range of applications, particularly in photocatalysis systems. In this presentation, we delve into the current advancements in the design and synthesis of CTFs, with a particular focus on their applications in photocatalysis. The discussion begins with a brief overview, tracing the historical development of photocatalytic research areas. Subsequently, various synthetic strategies employed in the creation of CTFs are detailed and compared. The presentation further explores the progress of CTF materials in the realm of photocatalysis, highlighting strategies aimed at enhancing their photocatalytic performance. Lastly, we consider future perspectives and challenges, addressing the synthesis of high crystalline CTFs and the design of CTF materials with outstanding catalytic capabilities [2]. This discourse aims to inspire further advancements in the application of CTF materials in photocatalytic processes.

Keywords: Covalent triazine framework; Photocatalytic application; Dye degradation; Water purification; Porous organic material



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Design of a solar cell based on simulations of InAlN semiconductor nanostructures

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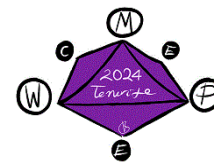
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In the present work, a preliminary study is carried out in order to design a solar cell based on simulations of semiconductor nanostructures which have previously been experimentally synthesized first in thin layers of InAlN using the Magnetron Sputtering RF technique, which are sought simulate using wxAMPS and python to analyze the optical and electrical response of the material and thus characterize it with its electrical contacts, by depositing the anterior and posterior layers based on different metals such as gold (Au), silver (Ag), copper (Cu) o Aluminum (Al), and other materials such as ITO, respectively, in order to examine the influence of these layers on the InAlN composite and thus achieve good solar cell efficiency.

Keywords: Solar cell, Semiconducting Nanostructures, Magnetron Sputtering, electrical contacts.

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Improved photocatalytic performance of lead-free organic-inorganic hybrid perovskites in H₂ production

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Lead-free halide perovskites have emerged as promising photocatalysts for energy and environmental applications such as H₂ evolution, CO₂ reduction and pollutant degradation [1]. In this regard, bismuth-based perovskite materials exhibit excellent stability under ambient conditions and remarkable physical-chemical properties [2], making them potential green photocatalysts. However, the use of these perovskite materials for photocatalysis in aqueous solution is limited due to their intrinsic instability in water. Thus, there is a need to develop new bismuth-based perovskites with enhanced water stability and efficient photocatalytic performance.

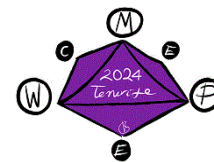
With this in mind, we prepared robust hybrid bismuth perovskites as photocatalysts for the gas-phase overall water splitting (OWS) reaction. For the first time, bismuth-based perovskites (named IEF-15, IEF-16 and IEF-17 for IMDEA energy framework) demonstrated significant photocatalytic activity in both H₂ and O₂ evolution [3]. To improve the H₂ photocatalytic performance of these materials, we propose an easy strategy to synthesize water-stable perovskites by alkylating the organic cations. To accomplish this, we used a facile solvothermal method to perform in-situ alkylation of a bulky diammonium cation, achieving the material denoted IEF-19-Pr. The results showed that IEF-19-Pr exhibits better water stability than the material containing the non-alkylated cation (IEF-19).

Acknowledgements

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Photocatalytic activity of TiO₂ nanorods on spherical FTO granules

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Most of the photocatalytic materials have efficiency and better surface reactivity compared to their bulk states in low dimensions due to increased surface area to volume ratio. The space charge region modulation becomes prominent on small crystalline materials [1]. In some cases, the growth of well-structured nanostructures on a supporting substrate requires the use of seed layers. For instance, prior to growing TiO₂ nanorod arrays, it is common practice to pre-coat the substrate with nanocrystals [2]. Recently, Hashitha et al. proposed seed assisted thermal oxidation method to trigger TiO₂ nanowires formation under controlled atmosphere [3]. Among synthesis methods of TiO₂ nanostructures, hydrothermal has been favored the most due to its low cost, low-temperature operation, and environmentally friendly nature [4].

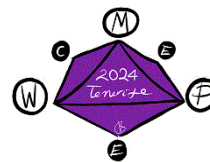


In this study, we investigated TiO₂ nanorod formation on spherical FTO granules (Fig. 1) to enhance the photocatalytic activity accelerating the charge transfer by the creation of large surface area to contact with dye molecules and boosting the light harvesting by enlarging the substrate dimension from 1D to 3D. After experiencing the precursor effect on the FTO seed layer formation on flat glasses by dip-coating method and confirming non-axial growth of TiO₂ nanorods on semi-spherical FTO islands, the selected solutions were used for spray dry to fabricate fully spherical FTO granules.

Figure 1. TiO₂ nanorods on FTO granules.

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Unleashing the potential application of direct ammonia fuel cells

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The difficulty of pure hydrogen storage has been a motivation to develop new systems based on intermediate species that have a high hydrogen storage capacity and, at the same time, are most easily stored and transported. [1,2]

Direct ammonia fuel cells (DAFC) are a type of fuel cell based on the ammonia oxidation reaction (AOR) in the anode and the oxygen reduction reaction (ORR) in the cathode. These systems need to work in alkaline media because ammonia, at low pH, can be found as ammonium which is so inactive and requires high potential for its oxidation. [3]

The catalysts used so far for AOR can be organized into two groups: Pt-based electrocatalysts and Ni-based electrocatalysts. The problem with Pt-based materials is that not all facets are active to oxidize the ammonia only the Pt(100) facet contributes to the oxidation of NH₃, however, it is quickly deactivated due to the irreversible absorption of N [4]. Thus, Ni appears as an alternative to platinum because it is intrinsically satisfactory for NH₃ dehydrogenation and it exhibits significantly promising long-term stability for a few hours [4]. By the other side, materials which contain Ni and Cu have demonstrated a good performance for the AOR showing morphology dependence. [5]

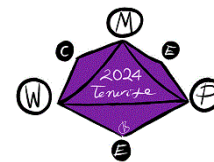
In my PhD thesis, it is proposed the synthesis of materials based on Ni with different morphology to perform the AOR. The work is focussed on the production of Ni-MOFs and Ni hydroxide which can be doped with Cu to increase the selectivity of ammonia oxidation to nitrogen. For the ORR, MOFs materials have been selected, that can be used as directly as catalysts or as precursors to produce single atoms catalysts from them.

Acknowledgements

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MXenes as catalysts for hydrogen evolution reaction

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Hydrogen is considered an energy vector for the transition to more sustainable energy sources. Electrolysers allow the production of high-purity H₂, easing its use in fuel cells. Platinum group metals (PGM)-based materials are usually employed as electrodes in both water electrolysers and fuel cells, since they exhibit high performances. A well-known drawback associated to these materials is their high cost and scarcity, forcing the designing of novel catalysts with low/zero content of PGMs. Transition metal carbides emerge as an alternative to these metals due to their good catalytic activity for electrochemical hydrogen generation [1,2].

This work presents the results obtained for the hydrogen evolution reaction (HER) on three-dimensional carbides (commercial) and two-dimensional carbides (MXenes). MXenes have been synthesised by selectively removing the "A" metal from their precursor compound, called MAX phase, with a general formula M_{n+1}AX_n, where M is a transition metal, A represents an element mainly from groups 13 and 14, carbon or nitrogen as X, with n = 1, 2, 3.

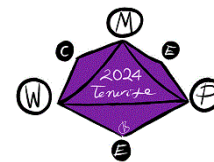
All materials have been physicochemically characterised using X-ray techniques (diffraction, XRD; energy-dispersive spectroscopy, EDX), microscopic techniques (scanning electron microscopy, SEM; transmission electron microscopy, TEM), and Raman spectroscopy. The electrochemical response towards HER has been evaluated through cyclic voltammetry, linear sweep voltammetry, and electrochemical differential mass spectrometry (DEMS), which has allowed a deeper understanding of the mechanistic aspects of this process [3]. MXenes exhibited suitable catalytic activities towards HER, with a lower overpotential for evolution compared to their precursors and commercial 3D carbides.

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Electrolytes with weberite structure based on

$\text{La}_{3-x}\text{Ca}_x\text{NbO}_{7-\delta}$ for application in power conversion devices

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Polycrystalline powders of $\text{La}_{3-x}\text{Ca}_x\text{NbO}_{7-\delta}$ ($x = 0, 0.1$ and 0.2) have been prepared by a freeze-drying precursor route to study their properties as proton conducting materials [1]. The phase formation and evolution with the temperature was studied by X-ray diffraction (XRD). The microstructure of sintered pellets was examined by scanning electron microscopy (SEM). Dense ceramic materials were obtained at $1400\text{ }^\circ\text{C}$ and the different contributions to the overall conductivity, bulk, and grain boundary, were studied using impedance spectroscopy under different atmospheres and the effect of calcium dopant on electrical properties of lanthanum niobates was analyzed. The equivalent circuit generally used to fit the impedance spectra of Ca-doped samples can be basically associated with a resistance in parallel with a capacitor, while

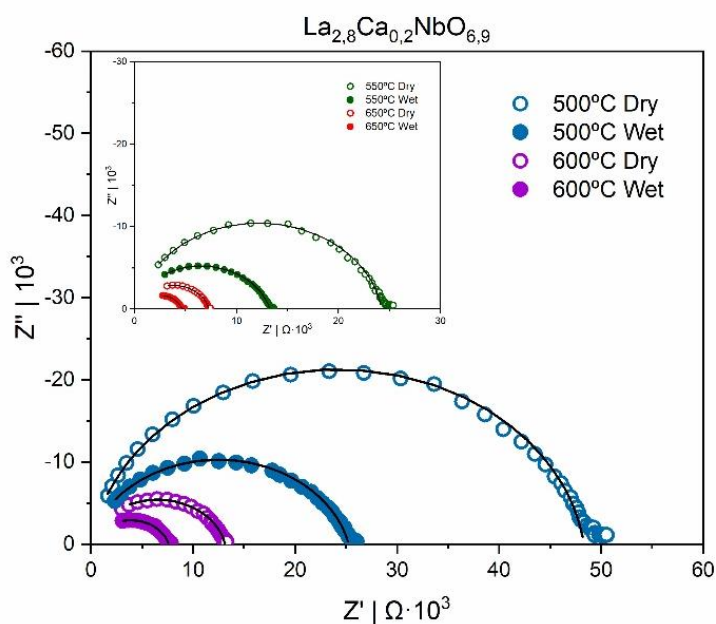
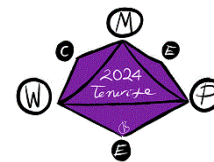


Figure 1. Impedance diagrams for dense $\text{La}_{2.8}\text{Ca}_{0.2}\text{NbO}_{6.9}$ pellets sintered during 24 h on wet and dry air.

the semicircle corresponding to the grain boundary processes does not appear, indicating the homogeneity of the doped samples (Figure 1). It should be noted that, the conductivity increases with the calcium content, due to the increase in concentration of structural oxygen vacancies caused by the presence of the dopant. Also, we should mention that the generation of oxygen vacancies involves the existence of interstitial proton defects and, therefore, the conductivity increases when the gases used are humidified [2]. In this sense, these materials can be considered proton conductors [3].

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Zn_{1-x}Cd_xS/TaON for photocatalytic water splitting

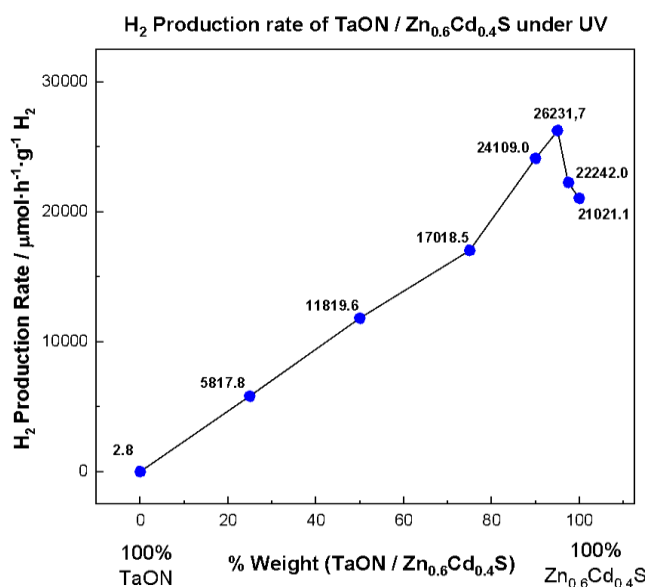
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Green hydrogen production by water splitting using photocatalytic semiconductors allow the split of water into hydrogen and oxygen using solar radiation [1]. However, quick recombination of charge carriers and photocorrosion limit the activity and application of these materials[1]. Combination of semiconductors with different band gaps could lead to a direct Z-Scheme heterojunction that prevent electron hole recombination and increase the hydrogen production rate by photocatalytic water splitting [2].

In this work, we present Zn_{1-x}Cd_xS/TaON heterostructure with high hydrogen production rates by photocatalytic water splitting. TaON was synthesized by ammonolysis method using Ta₂O₅ as precursor at 850 °C under flow of NH₃ gas. Zn_{1-x}Cd_xS was prepared by an aqueous green method at room temperature in water, leading to a sphalerite structure. The heterostructure in different weight percentage of both materials was achieved by precipitation of Zn_{1-x}Cd_xS over TaON at room temperature. The structure, morphology and band gap energy of the materials were studied by X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-Vis diffuse reflectance spectroscopy respectively. Photocatalytic water splitting measurements were performed under UV and Visible radiation in a borosilicate jacketed-reactor with a thermostated water circulation system. Typical photocatalysis experiment was carried out using Na₂S/NaSO₃ as sacrificial agent under constant stirring at 20 °C. The continuous hydrogen production rate was determined by a mass spectrometer connected to the reactor output.

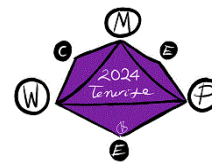


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Electrolytes with pyrochlore structure based on the $\text{La}_{2-x}\text{Ca}_x\text{ScNbO}_{7-\delta}$ for application in solid oxide electrolyzers (SOEC)

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Solid Oxide Electrolyser Cell (SOEC) are defined as electrochemical devices that usually produce oxygen and hydrogen, by splitting the water molecules. The SOECs can be described as Solid Oxide Fuel Cells (SOFCs) working in a regenerative mode, which require an external electrical current. They work at high temperature (typically 600-800°C). The most studied SOECs are those that use ceramic materials such as YSZ or CGO as electrolytes [1]. Their main advantage is the high operating temperature, that improve the efficiency power-to-hydrogen, reducing the cost of hydrogen production. If renewal energy is supplied the hydrogen produced is green.

This work focuses on the development of new proton conducting ceramic materials (PCCs) that can be used as electrolyte [2] in this type of cells, decreasing the operating temperature, giving raise to intermediate temperature solid oxide electrolyzers (IT-SOEC). Materials with composition

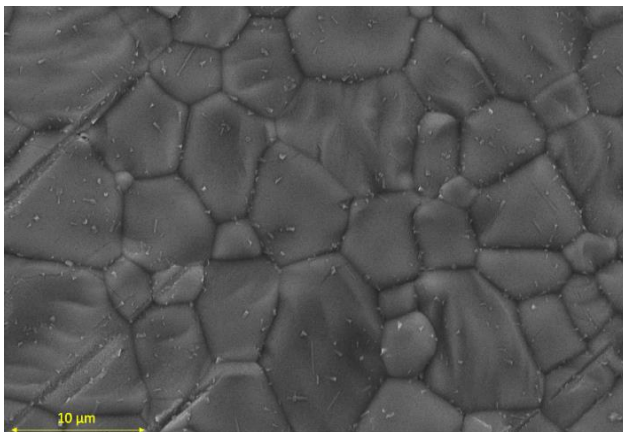
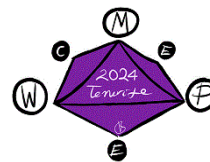


Figure 1. SEM image of the sample $\text{La}_2\text{ScNbO}_7$ after sintering process.

$\text{La}_{2-x}\text{Ca}_x\text{ScNbO}_{7-\delta}$ where $x = 0.00; 0.025; 0.05; 0.075$ and 0.1 , were synthesised by freeze-drying precursor method; and structural and morphologically characterised by XRD and SEM. The ionic/electronic transport properties were determined by complex impedance spectroscopy (EIS) [3], in the temperature range of 200-900°C, and in the presence of different dry and wet gases (Air, Argon, 5% H_2 in Argon). It has been shown that this family of materials exhibits proton conductivity, which were explained in terms of the Grotthuss mechanism.

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Photocatalysts for environmental applications

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Photocatalysis is an emerging area of chemistry that uses light as the primary energy source to carry out chemical transformations.

Although semiconductors such as TiO₂ have been extensively studied as photocatalysts, no commercial TiO₂-supported photocatalyst is used for wastewater remediation. Hence, we present herein a novel TiO₂-supported photocatalyst composed of titania-covered glass wool (GW) fibers decorated with SiO₂-TiO₂ core-shell spheres. For optimizing the photocatalytic activity of this material, the surface of SiO₂ microspheres, as well as the highly mechanically resistant GW fibers, were covered by an optimized layer of TiO₂ (ca. 20-30 nm), containing nanometric crystals of ca. 12 nm linked between them and to the surface of SiO₂ microspheres and to the GW (Si-O-Ti). Its photocatalytic activity was evaluated against the recalcitrant pollutant phenol under a continuous flow in a solid-phase stationary photoreactor coupled to an *in situ* TOC detector. The complete mineralization of phenol was produced in less than three minutes, without titania leaching. Therefore, this photocatalyst has been demonstrated to be suitable for the industrial scale-up of wastewater treatment, in flow photoreactors at the plant scale.[1]

Moreover, organic photocatalysts appear as an alternative that has proven to be efficient in treating polluted effluents under visible light. Furthermore, their heterogenization seems the straightforward step to boost photostability and facilitate recovery after the reaction. To demonstrate this alternative, we have developed a strategy to covalently anchor an anionic photosensitizer (Rose Bengal, RB) together with cationic chains on GW, in a single reaction step to obtain a new GW-RB⁺ photocatalyst. As a result, this novel heterogeneous material showed a high efficiency in the photoinactivation of Gram-positive bacteria, but more interestingly, it also produced the inactivation of the refractive *E. coli* (Gram-negative). It has been demonstrated that this dual design, which includes the cationic chains and RB, causes a synergistic effect that was crucial to producing the photoinactivation of Gram-negative bacteria. In fact, control experiments using GW-RB as a photocatalyst without cationic chains only produced the photoinactivation of Gram-positive, but it was completely inactive to *E. coli*. Thereby, the cationic charges of GW-RB⁺ fulfil two functions, their own bactericidal action and enhance the activity of RB, which is mainly produced by the generation of singlet oxygen. Moreover, GW-RB⁺ and GW-RB were efficient in water decontamination, as demonstrated using diclofenac as a model compound. The synthesis of this kind of dual photocatalyst opens the path for efficient antimicrobial photoinactivation of multi-resistant pathogens and can be used for the development of self-disinfecting surfaces in all types of silica-based materials.[2]

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reaCtor: Optical fibre plasmonic microreactor for flow chemistry

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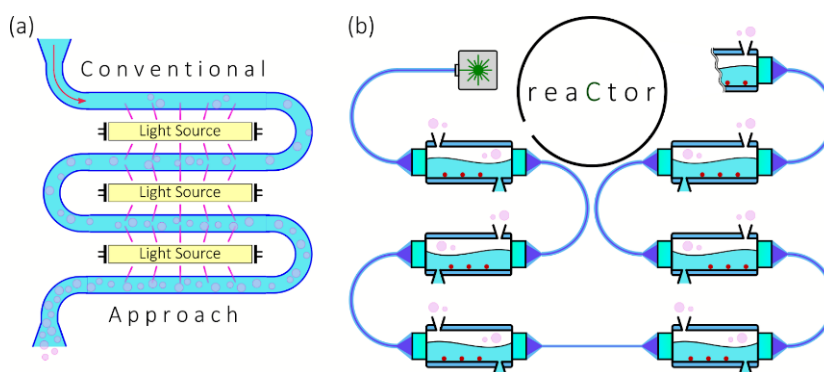
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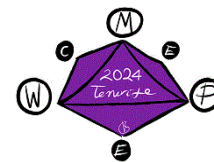
The chemical industry is a major contributor to CO₂ emissions as it accounts for about 30% of industry's total energy use worldwide. Thus, disruptive technologies are needed to reduce its greenhouse gas emissions. Photochemistry in flow microreactors promises to sustainably produce chemical compounds and has received a lot of attention due to the prospect of utilizing

(sun)light to drive these reactions. Still, the technique has not been widely used due to a challenging light management which hinders large-scale application in industry. This is exactly where reaCtor initiative comes into play by offering an



innovative solution: microreactors will be integrated inside a specialty optical glass fiber, where laser light is coupled in and the chemical reaction is enhanced by plasmonic nanoparticles, which locally amplify the optical field of the incoupled light. This approach allows to use a single light source for multiple reactors, thereby enabling a huge scale-up potential towards a sustainable chemical industry. Our goal is to set-up a demonstrator and benchmark it with photocatalytic reactions. reaCtor is a European Innovation Council (EIC) programme project (GA101099405) starting in May 2023. In this flash presentation we will show the main key ideas of the project which present a novel technology within the areas of photonics for energy and chemistry.

The project reaCtor has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No. 101099405.



Heterostructures of β -TaON with TiO_2 for hydrogen production by water splitting

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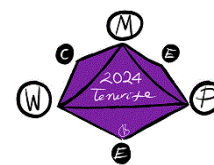
Since the beginning of this century a hydrogen economy has been proposed to solve the problems that fossil fuels have been causing to our planet.[1] Green hydrogen is a vital tool for achieving carbon neutrality, revolutionizing energy with its clean and versatile applications. It stands as a beacon in the transition to a more sustainable and eco-friendlier world.

The interest of using β -TaON in photocatalytic water-splitting is that the oxynitrides of Tantalum have absorption edges at 500–600 nm corresponding to bandgap energies between 2,0 and 2,5 eV. Due to these bandgap excitations, they work as photocatalysts for H_2 evolution from aqueous solutions. [2]

We have prepared β -TaON by ammonolysis using Ta_2O_5 as a starting reagent at 850°C, for 3 hours under a flow of 100 mL/min of NH_3 gas saturated in water.[3] The deposition of the TiO_2 nanoparticles was performed by dropping a solution of Titanium (IV) isopropoxide over a β -TaON aqueous suspension. The material obtained was characterized by X-Ray Diffraction, Diffuse Reflectance Spectroscopy and SEM. The photocatalytic measurements were performed under Visible and UV radiation. A borosilicate double-wall reactor with a thermostatic water circulation system was used with methanol as a sacrificial electron donor with constant stirring. The continuous production rate was determined using a mass spectrometer connected to the measurement equipment.

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Synthesis, characterization and catalytic properties for the ethanol transformation of La-Mg hydrotalcites

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Ethylene is considered a key feedstock for the chemical industry [1], and traditionally it has been synthesized by steam cracking (high-energy cost). So, is necessary to develop an alternative less expensive and eco-friendly. Is possible to obtain ethylene from the dehydration reaction of ethanol produced in sugar platforms for the transformation of lignocellulosic biomass from agricultural waste.

In this work, MgO/La₂O₃ catalysts were prepared. The catalysts were studied in the ethanol gas-phase conversion.

Table 1. Reaction conditions: 5 v/v% EtOH in N₂, T_R: 400°C, WHSV: 0.30 g EtOH/(g_{cat}·h).

Sample	Conversion, Selectivity (%)							
	EtOH	Acetalde-hyde	1-Butanol	Butenes	Ethylene	CO ₂	Higher Alcohols	Ketones
MgO	20.4	30.7	23.5	11.8	16.0	1.0	5.2	3.9
Mg/La=4	74.4	4.2	3.0	6.8	57.8	10.0	0.0	13.6
Mg/La=3	75.4	4.6	4.0	6.7	51.9	10.0	0.0	16.1
Mg/La=2	72.4	1.6	0.9	5.1	77.5	6.0	0.0	4.4
Mg/La=1	84.2	1.0	0.1	4.9	87.0	4.0	0.0	1.6
La ₂ O ₃	28.9	5.9	0.8	-	72.8	4.0	0.0	10.6

The excess of Mg in the catalysts drives to the formation of acetaldehyde/1-butanol, by a Guerbet mechanism. Surface analysis showed that the pore volume increases with Mg content. The same trend was observed when studying the basicity by CO₂-TPD: the density of basic sites increases due to MgO (weak strength), while stronger basic sites are attributed to the presence of La₂O₃. XPS and XRD revealed that the La₂O₃ catalyst is more prone to suffer carbonation. The progressive incorporation of Mg-species diminishes the trend to carbonation. The analysis of C1s core level spectra of the used catalysts showed a new contribution assigned to C-OH or C-O-C bonds. This signal could be ascribed to the adsorption between the basic sites with the alcohols.

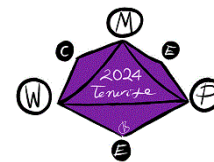
The La₂O₃ sample displayed narrower peaks (XRD): (higher crystallinity and lower porosity).

Acknowledgements

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CeO₂ - TiO₂ nano-octahedra as active photocatalysts for ciprofloxacin photodegradation under solar light

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Advanced Oxidation Processes (AOPs) involve the in-situ generation of short lifetime reactive oxygen species (ROS), like OH radicals, which are highly oxidative, electrophilic and non-selective species able to oxidize a wide variety of recalcitrant and toxic compounds [1]. Among all, photochemical AOPs combining the use of a photocatalyst, and light irradiation have arisen as one of the most promising alternatives for the removal of pollutants in wastewater. Titania (TiO₂), an n-type semiconductor, is the most studied and exploited photocatalyst for UV-based AOPs operating under mild conditions [2].

In this work, ceria-doped titania nano-octahedra (CeTNOh) were synthesized through ultrasonication-hydrothermal treatment using Ce-containing titanate nanowires derived from commercial titania (Degussa P25) with varying Ce content (0.75-1.5 wt.%) and tested in ciprofloxacin photodegradation under solar light irradiation.

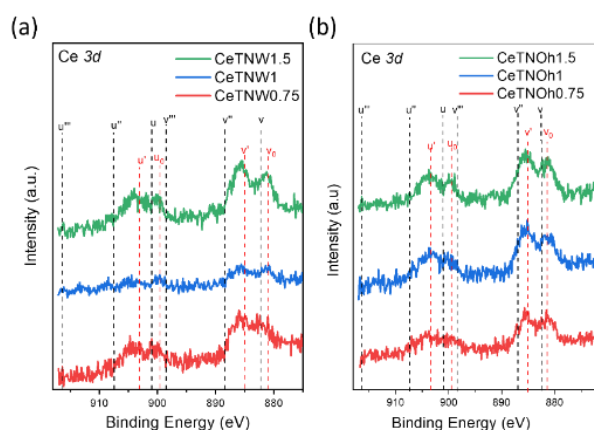


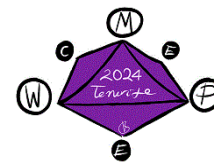
Figure 1. Ce 3d core level spectra for the prepared samples.

All samples exhibited anatase polymorphs. Hydrothermal treatments yielded nanowires and nano-octahedra with enhanced specific surface area compared to commercial P25 titania, though a decrease was observed with added Ce. HR-TEM images confirmed the desired morphology, with higher Ce concentrations impeding complete transformation from nanowires to nano-octahedra. XPS analysis revealed Ce³⁺ and Ce⁴⁺ species (Figure 1), enhancing electron mobility and facilitating Ti-Ce interaction.

UV-Vis spectroscopy indicated a reduced band gap with increasing Ce loading. The most effective sample achieved an 83% ciprofloxacin removal after 360 minutes of simulated solar light exposure, with minimal dark adsorption. Ce loadings exceeding 0.75 wt.% adversely affected photocatalytic performance, suggesting a promoting role for Ce but hindrance beyond optimal concentrations. Reusability tests with the most photoactive sample, CeTNOh_{0.75}, demonstrated robust stability and sustained photoactivity over three cycles.

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Evaluation of photocatalytic mortars in a real environment.

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One of the most critical environmental problems in urban settings is the air pollution by NO_x gases, which are originated from the combustion of fossil fuels, primarily in heating systems and road traffic. Photocatalysis has been proven to be a successful pathway to alleviate the impact of these gases on the pollution of cities, simply by incorporating photocatalysts into construction materials (concrete, mortars, bricks, ceramic, etc.). The functioning of these materials is extensively studied at the laboratory scale, however, only a few studies have contrasted their performance at a real scale, been negligible those conducting simultaneous in situ measurements of photocatalytic materials.

On the other hand, the most widely used photocatalytic material in construction mortars is TiO₂. This material has certain advantages, such as its band gap and excellent performance with UV light radiation. However, it has drawbacks including poor selectivity in the photochemical oxidation process of NO gases and limited performance under visible light conditions. To address these drawbacks, we have developed alternative photocatalysts based on LDHs (Layered Double Hydroxides) that exhibit efficiency equal to or greater than that of TiO₂ and significantly improved selectivity, in addition to enhancing their performance in the visible spectrum. [1,2].

Four mortar panels with different photocatalytic additives (reference, TiO₂, NiTi-LDH and ZnCr-LDH) were placed near to the highway at the entrance of a 200 m tunnel, as it is shown in the Figure 1.



Figure 1. Placement of the panels

Tabla 1. Conversion values for the different panels

		Removal gases (%)		
		T1 07:00- 14:00	T2 14:00- 19:00	T3 19:00- 22:00
TiO ₂	NO	74	60	61
	NO ₂	59	70	71
	NO _x	65	69	71
LDH- NiTi	NO	21	50	53
	NO ₂	85	76	94
	NO _x	40	65	71
LDH- ZnCr	NO	36	31	54
	NO ₂	91	85	91
	NO _x	50	51	76

The experiment was conducted by continuous measurement using two simultaneous NO_x gases analyser instruments. One of them remained operational throughout the experiment, monitoring the reference mortar, while the other alternated on a weekly basis to

assess the photocatalytic activity of each of the other 3 studied mortars.

The profiles obtained over a 24-hour period are presented in Figure 2, corresponding to the mortar with ZnCr-LDH. The average data for the 3 mortars are detailed in Table 1.

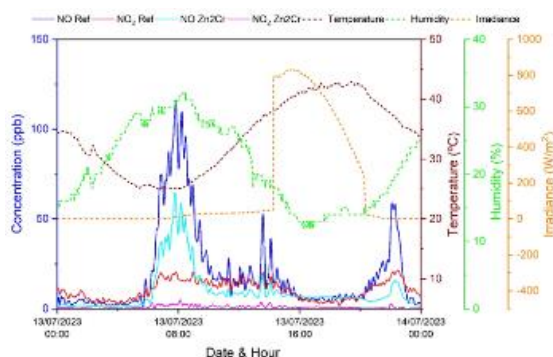
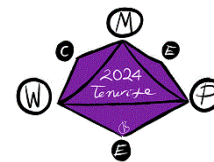


Figure 2. Daily NO_x gases concentration measured

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Hypercrosslinked polymers as potential catalysts for biodiesel production

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The escalating global interest in biodiesel as a sustainable alternative to fossil fuels has underscored the need for efficient and cost-effective production methods. Transesterification stands out as the predominant approach due to its simplicity and favorable biofuel characteristics. However, challenges persist in reducing production costs, necessitating the exploration of diverse feedstock sources. Extensive research on heterogeneous catalysts, particularly metal oxides, has been conducted [1], yet obstacles such as the requirement for high-quality waste oils and issues related to catalyst reusability. This study presents an innovative solution to these challenges by introducing a hypercrosslinked polymeric (HCP) catalyst with basic active centers, synthesized through a sustainable mechanical polymerization process. While porous organic polymers (POPs) are renowned for their unique properties, their application in basic catalysis for biodiesel production represents a novel contribution.

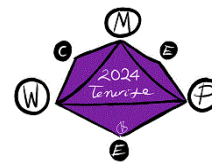
Exploring the basic character of catalyst hypercrosslinked polymers (HCP-K), this study demonstrates its efficiency in transesterification reactions using feedstocks of diverse origins and qualities. Analysis of critical properties of biodiesel feedstocks, including acid value, viscosity, and density, provides insights into their impact on the transesterification process. The HCP-K catalyst exhibits exceptional catalytic activity, achieving an 99.9% FAME content with two hours of reaction time. Additionally, the study investigates the influence of free fatty acid (FFA) content on FAME yield, highlighting the catalyst's ability to perform effectively with oils containing moderate FFA levels. This research contributes valuable insights to the field, paving the way for sustainable and efficient biodiesel production.

Acknowledgements

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Efficient MXenes@TiO₂ composites for photocatalytic gas phase degradation and reduction processes

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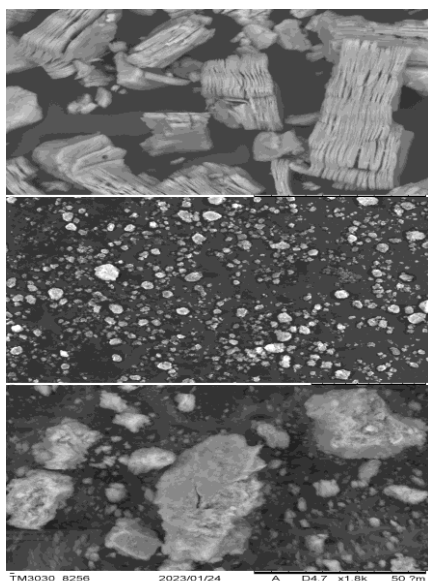
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MXenes (two-dimensional (2D) transition-metal carbides, nitrides, and carbonitrides) have several excellent properties such as metallic conductivity and hydrophilicity [1]. Consequently, there is a growing interest in MXene-based photocatalysts. The formation of these composites is due to the electrostatic self-assembly between positively charged photocatalysts and negatively charged MXenes [2].

In this work, several composites based on Ti₃C₂ and different types of TiO₂ were synthesized. These materials were tested in the following gas-phase reactions: the degradation of 1-butanol and the photocatalytic reduction of CO₂.

The composite Ti₃C₂@P90 that contained 10 % of MXene was the most efficient both in the degradation of 1-butanol and in the reduction of CO₂.



The Ti₃C₂, the different TiO₂ employed in this work and the synthesized composites were characterized by Aggregate distribution and Scanning Electron Microscopy, X-Ray Diffraction, and N₂ adsorption analyses (BET-BJH).

The Figure shows SEM images of the synthesized Ti₃C₂ (A), commercial TiO₂ (P90) (B) and the Ti₃C₂@P90 composite (C).

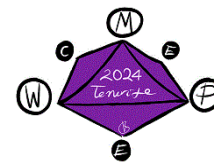
FTIR studies of the interaction and degradation of 1-butanol in the gas phase revealed a highly negative surface charge of Ti₃C₂@P90 that inhibits the formation of carboxylates on the surface of the catalyst; this avoids deactivation processes, promotes the degradation of intermediates and facilitates the separation of the photogenerated e⁻/h⁺ pairs.

Acknowledgments

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Green and sustainable biodiesel Production: Utilizing adsorption and heterogeneous catalysis

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The industrial production of biodiesel commonly involves transesterification of triglycerides from vegetable oils using methanol and basic homogeneous catalysts, such as NaOH or KOH. However, this process has limitations, including the need for post-synthesis separation steps, inability to use high free fatty acid (FFA) content raw materials, and non-reusability of the catalyst. To address these issues, the use of heterogeneous catalysts is being studied as an eco-friendly and cost-effective alternative. This research aims to produce biodiesel sustainably by subjecting oils to adsorption, instead of esterification, to reduce high FFA content and then transform them into biodiesel using heterogeneous catalysis. The goal is to make the biodiesel production process more environmentally friendly, reducing operational and maintenance costs.

The study involved obtaining and characterizing two types of residual frying oils. An adsorbent made from *Pongamia pinnata* shells [1] was synthesized and used to remove FFAs present in residual frying oils, eliminating the need for the esterification reaction. A heterogeneous catalyst (Li/Pumice) [2] was utilized for the transesterification reaction, which was compared with conventional homogeneous transesterification.

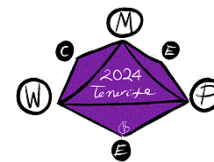
The study showed that Li/Pumice catalyst has economic and environmental advantages by using a natural, abundant, and low-cost material, reducing soap formation and effluents. The content of FFAs in the waste oil influences the quality of the produced biodiesel. The use of an adsorbent synthesized from *Pongamia pinnata* shells instead of sulfuric acid for reducing FFA content contributes to a more sustainable biodiesel production process. The process combining adsorption with homogeneous and heterogeneous transesterification produced biodiesel with high FAME (fatty acid methyl ester) content. The study demonstrates the feasibility of producing biodiesel from used cooking oil in a more efficient and sustainable manner.

Acknowledgements

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Photoreforming of biomass derivatives for Hydrogen generation. Use of Cu/TiO₂ and Cu/TiO₂-C photocatalysts

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The high energy demand and the current model based on fossil fuels is becoming a serious problem that reveals the necessity of alternative and clean fuels and the so-called green hydrogen can be a very suitable option. In this context, the present work deals with the photocatalytic generation of hydrogen by the photoreforming of biomass or biomass derivatives, like cellulose, using TiO₂-based photocatalysts [1]. In order to improve the efficiency of bare titania, it has been modified with carbon and/or with copper.

A series of bare titania and carbon-doped titania photocatalysts were prepared by hydrothermal synthesis of TiO₂ (12 h, 180 °C) using either sucrose [2] or graphene oxide as carbon sources. Copper was incorporated to the TiO₂ and TiO₂-C samples by impregnation with an aqueous solution of copper nitrate [3]. Analogous samples prepared with the commercial titania P25 were also tested. The prepared catalysts were characterized using several techniques (ICP-OES, XRD, XPS, and TEM). The photocatalytic activity tests were performed in a 1L Heraeus UV-RS-2 glass reactor with a 150 W mercury lamp (365 nm). The biomassic substrates used are cellulose, almond shell and the residual liquid of hydrothermal carbonization of almond shell. The generated gas was swept by He flow (60 mL/min) and continuously analysed by mass spectrometry.

XRD data show that anatase is the main crystalline phase of the synthesized TiO₂. XPS results reveal that copper is mainly present as Cu(I) and/or Cu(0). The tested photocatalysts show, in general, a high hydrogen production, being the catalyst that contains carbon (from sucrose) and copper the most active one. The activity of these catalysts for hydrogen generation is noticeably higher than the one determined for the commercial titania P25 [3]. The obtained results show an important effect of both, carbon doping and metal incorporation, in the photocatalytic performance of TiO₂.

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P- 08

On the need of new materials for pressure retarded osmosis

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Pressure retarded osmosis is a membrane-based renewable energy source based on the controlled mix of two streams with different salt concentrations (such as river and sea water) [1,2,3]. It has been extensively demonstrated at lab level, but several bottlenecks are hindering the deployment in real installations. In fact, validations using real-life data indicate that improvements in several sections are needed [4].

Among the improvements needed is the performance of the materials of the membranes, which are integral part of controlling the mix (see schema in Figure 1 [5] and some numbers for a proposed case study in Figure 2). Multiple attempts to improve the materials are being proposed, showing some improvements when, for instance, surface treatments are used in commercial membranes [6,7,8]. However, further improvements are needed in these materials if the process is to be implemented in industrial practice: this is an open problem that is worthy of study.

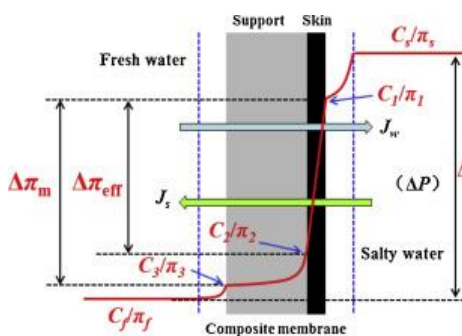


Figure 1. Concentrations in PRO process [5]

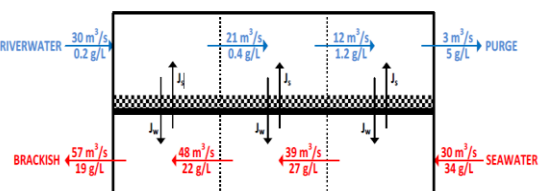
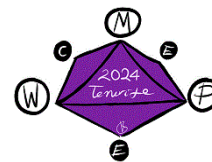


Figure 2. Expected flows in a proposed application

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Biopolymers as sorbents for the extraction of persistent and emerging contaminants from wastewater

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Biopolymers are materials obtained from natural sources that have the potential to be a sustainable alternative to traditional polymers in many applications [1,2]. Among them, it is important to highlight their use for adsorption, removal, and determination of pollutants from aqueous media. Most of the reported studies developed with these endings requires of biopolymer functionalization or combination with other materials to create composites. These procedures in general entail the use of organic solvents and requires of the use of expensive reagents and long synthetic procedures. There is a need for alternative studies able to directly use unmodified biopolymers for the extraction of pollutants.

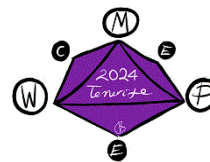
This study explores the use of unmodified biopolymers, specifically from the polysaccharide (chitosan, agarose, and cellulose) and protein (keratin) families, as sorbents. These materials were applied for the extraction of environmental contaminants such as polycyclic aromatic hydrocarbons (PAHs) and personal care products from wastewater. The use of biopolymers in this context aligns with the current trends in Green Chemistry. In addition, keratin provides high efficiency for the adsorption of these two families of pollutants.

Acknowledgments

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Multicomponent metal-organic frameworks for adsorption of organic pollutants

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Since the first report on the synthesis of a metal-organic framework (MOF) [1], numerous porous crystalline materials formed by the combination of metal clusters and organic linkers (secondary building units, SBUs) have been created by a lot of methods, and showing great diversity of topologies, surface areas, and pore size distributions. Consequently, MOFs are being applied in a variety of fields, including catalysis, energy storage, drug delivery, and pollutant adsorption [2]. However, the implementation of these functional materials into these applications demands their sophistication. In this sense, complex MOFs constituted from more than one type of SBU and termed multicomponent MOFs have been introduced. The possibility of varying the type of SBUs and their proportion offers the opportunity of controlling structural features of the final MOF, including pore size and surface area, thus increasing the tailoring control [3]. In this work, we study multicomponent MOFs constructed from a zirconium cluster and two different linkers (4,4'-(azobenedicarboxylic acid, abdc, and 2,6-naphthalenedicarboxylic acid, ndc): $Zr_6O_4(OH)_4[(abdc)_{1-x}(ndc)_x]_6(H_2O)_6$, where x takes values from 0 to 1 in steps of 0.1. These materials are synthesized and properly characterized. In addition, we study the adsorption behaviour of these MOFs in aqueous media by means of adsorption kinetics towards different organic pollutants.

Acknowledgments

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Chalcopyrite-based thermoelectric materials prepared by microwave-hydrothermal synthesis

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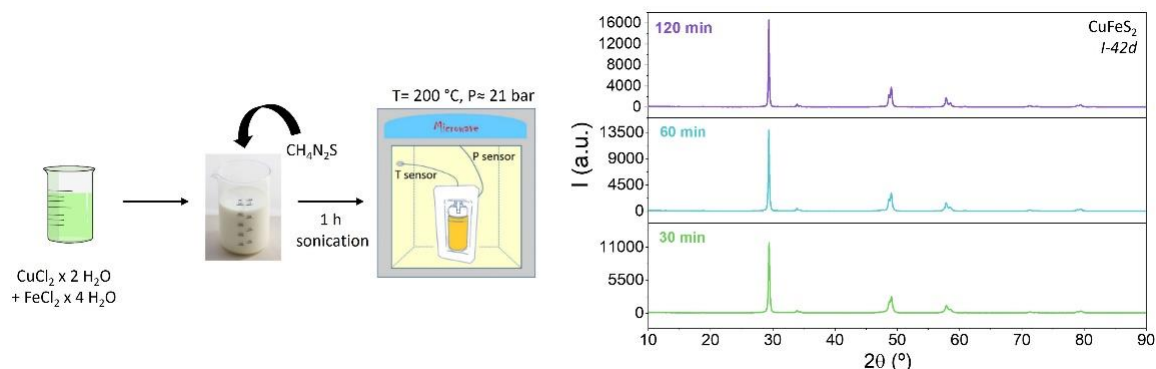
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The escalating global energy demand and the associated release of greenhouse gases have raised serious concerns regarding climate change. The substantial release of heat emissions resulting as a byproduct of human activities and natural processes present a significant environmental challenge. In this context, thermoelectric devices emerge as a promising solution to address both the recovery of waste heat and the quest for more sustainable energy sources, as they can convert waste heat into electrical energy. However, the limited conversion efficiency of existing commercial thermoelectric devices, coupled with the high toxicity and scarcity of constituent elements, poses challenges to their widespread adoption [1].

The n-type chalcopyrite, CuFeS₂, has garnered significant interest as a promising thermoelectric material due to its inherently low lattice thermal conductivity and the abundance of its non-hazardous and inexpensive constituent elements [2]. One of the most common synthetic routes to prepare this material is solid-state method [3]. Nevertheless, it has certain drawbacks such as the use of relatively high temperatures, working in vacuum conditions, high time consumption and the necessity of intermediate grindings.

This study focuses on optimizing the reaction time in the synthesis of polycrystalline CuFeS₂ phases by using microwave-assisted hydrothermal method. Additionally, structural and microstructural characterization, as along with the thermoelectric properties of the aforementioned phases will be presented.



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Metal-biohydrogels as green and heterogeneous catalysts in tandem reactions

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Alginate, a polysaccharide with the ability to form biopolymers through ionic reactions with metal cations, stands out in various applications, including the chemical and pharmaceutical industries, and specifically in catalysis.

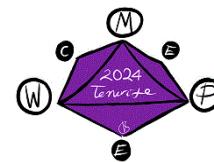
Currently, tandem reactions have gained popularity due to their advantages over traditional synthesis methods. These advantages include greater atom efficiency and the elimination of toxic by-products by avoiding purification and separation steps during synthesis.

In this study, alginate hydrogel beads (AHG), alginate xerogel beads (AXG) and alginate aerogel beads (AAG) cross-linked with metal cations (Ca^{2+} , Cu^{2+} , Co^{2+} , Ni^{2+} , Zn^{2+} , Fe^{2+} and Fe^{3+}) were synthesized to evaluate their catalytic activity and study their recyclability in the synthesis of nitroaldol (Henry reaction). The tandem reaction involves the synthesis of p-nitrobenzaldehyde from p-nitrobenzyl alcohol as an intermediate, using different oxidizing agents such as TBHP, H_2O_2 , and O_2 . The catalysts were characterized using various techniques, including FT-IR, TGA, ICP-OES, and FE-SEM. [1]



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Coating ink based on a light-curing polymer and a metal-organic framework for the removal of emerging contaminants

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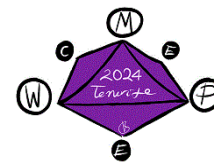
In recent years, the use of polymers for the develop of different composites has played a crucial role, mainly owing to their exceptional binding capabilities. Polymers are used in composites alongside an extensive array of materials like magnetic nanoparticles, covalent-organic frameworks, or metal-organic frameworks (MOFs), among others, and in many formats like particles or thin-film membranes.

For the preparation of thin films, a mixture of the monomer, the photoinitiator, and a reactive diluent is normally prepared and then coated onto a flat surface or solid support. Conventional polymers like polypropylene, exhibit a notable drawback during coating as solvent evaporation almost is the unique route to create the thin film. Therefore, investigating polymers responsive to stimuli represents a significant advantage for coating inks. In particular, certain light-responsive monomers initially are in a liquid state, but they solidify after polymerization, procedure that occurs upon exposure to UV light in the presence of a proper photoinitiator.

This study reports the preparation of thin-film membranes based on light-curing polymers and MOFs. We use glycidyl methacrylate and Darocure 1173 as monomer and photoinitiator, respectively, thus inducing photopolymerization through a radical reaction. In addition, MIL-100(Fe) is incorporated in the composite, MOF that have shown high efficiency as extractant materials for the removal emerging contaminants. The work shows the application of the prepared thin films for the removal of certain contaminants in water samples. Analyzing these contaminants is essential due to their classification as endocrine disruptors with the potential for bioaccumulation in organisms.

Acknowledgments

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Metal-organic frameworks for the extraction of bioactive compounds in aloe vera gel

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Metal-organic frameworks (MOFs) are crystalline materials consisting of metal ions or metal clusters and organic ligands linked by strong coordination bonds [1]. Their main characteristics depend on the selected organic ligands and their connectivity in the structure, together with their porosity, particle size, and nature of the metal cluster, among other factors. These materials are excellent sorbents for the extraction of organic compounds from aqueous media [1].

Aloe vera is a plant rich in bioactive compounds like phenolic compounds known as anthraquinones and chromones. The extraction of these compounds is of great importance in the cosmetic, food and agriculture industries.

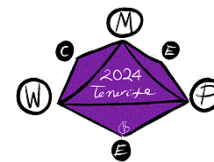
The aim of this study is to compare the efficiency of different MOFs, such as (Zr)-abdc and PCN-250 (Fe₂Co) for the extraction of bioactive compounds present in aloe vera gel.

Acknowledgments

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Composite materials synthesis and their application in pollutants extraction

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Parabens are a group of chemicals used in personal care. It is known that the bioaccumulation of these compounds causes great damage to human health and that is why there are numerous porous materials for their elimination (such as silica, zeolites, metal oxides, polymers, MOFs, etc.). Here we focus on metal-organic frameworks (MOFs), due to their great interest thanks to the ease of adopting and modifying their structure, offering precise control to select and capture different contaminants. In addition, these materials provide new properties, being able to improve their catalytic behavior. Through photocatalysis and adsorption processes, a selective decomposition is attempted to produce clean water. To this end, we propose the synthesis of MOFs compounds with photocatalysts in order to obtain new efficient photoactive materials. The selected photocatalyst was TiO₂ due to its high chemical and thermal stability, low production cost, non-toxicity and easy applicability in different environmental conditions.

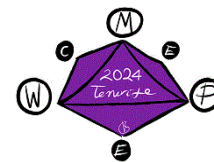
Different strategies were followed to integrate the photocatalyst and CIM-81, UiO-66, UiO-66-NH₂ as MOFs, in the new composite materials. Of the 15 synthesis carried out, 11 compounds could be obtained that were characterized by different techniques such as X-ray diffraction (XRD), thermogravimetric analysis (TGA), infrared spectroscopy (IR), dynamic light scattering (DLS), scanning electron microscopy (SEM) and N₂ adsorption. By studying the extraction capacity of the contaminants methylparaben (MPB), ethylparaben (EPB), propylparaben (PPB) and benzylparaben (BzPB) and their photoelectrochemical properties, a selection of 6 final compounds that presented a better photoelectric response was made.

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Graphene-based Ni catalysts as cathode for alkaline anion-exchange membrane fuel cells

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As the limited accessibility of conventional fossil fuels becomes more evident, the world needs to shift to more sustainable sources of energy. Therefore, the development of energy conversion technologies devices that provide clean energy (renewable and environmentally friendly), crucial to compensate for the expected shortage, has become key to alleviating this issue [1]. Extensive research in fuel cells (FCs) has demonstrated that doping graphene with N or S improves the catalytic activity of the catalyst, leading the reaction through the 4-electron pathway [2,3].

In this work, Ni nanoparticles supported on graphene-based materials were tested as catalysts for the oxygen reduction reaction (ORR) to be used in anion exchange-membrane fuel cells (AEMFCs), leading to robust durability results after 10 h, attributed to the synergetic effect of Ni nanoparticles and bi-doped (N,S)-reduced graphene oxide. As a result, these materials were found to be a promising alternative to the state-of-the-art Pt/C catalysts.

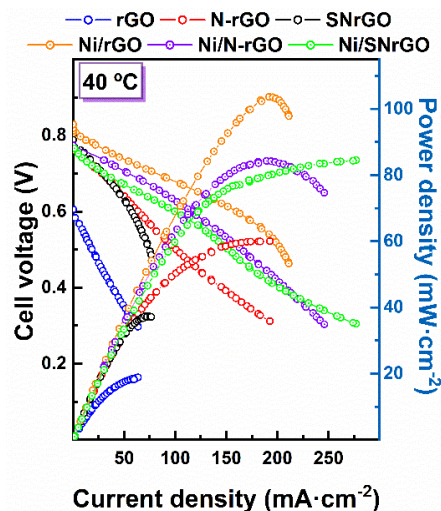


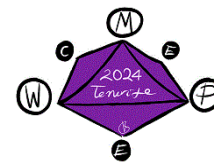
Figure 1. Polarization and power density curves for the as-prepared materials. FC performance data with the PtRu/C anode catalyst (0.35 mg·cm⁻² PtRu loading). H₂ and O₂ were supplied with flow rates of up to 0.5 and 1 L min⁻¹, respectively.

Acknowledgement

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Multivariate aluminum azobenzenedicarboxylate metal-organic framework (MOF) for the adsorption of pollutants in water

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Metal-organic frameworks (MOFs) are crystalline materials composed by metal ions or metal clusters combined with organic ligands [1]. These smart materials have been studied for a wide range of applications, such as gas storage and separation, catalysis, drug delivery, energy storage, and chemical sensing, among others [1]. Recently, multivariate MOFs built from more than one type of constituents (for example, two types of ligands) have been described with the aim of achieving new properties to exploit for the aforementioned applications [2,3].

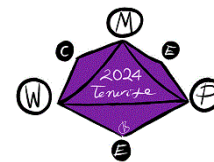
This work describes the synthesis and characterization of a family of multivariate MOFs based on Al(III) and two different organic ligands, namely 4,4'-azobenzenedicarboxylic acid (abdc) and 2,6-naphthalene dicarboxylic acid (ndc). These linkers have been combined in different ratios to synthesize Al-based MOFs similar to the CYCU-3 MOF previously reported [4]. The study also includes the application of the multivariate MOFs in the adsorption of a group of organic pollutants from aqueous samples.

Acknowledgments

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Metal-organic frameworks-based capillary stationary phases for the determination of emerging pollutants

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Metal-organic frameworks (MOFs) are crystalline materials composed of metal ions (or clusters) coordinated with organic ligands to create highly porous structures. They are known for their exceptional surface areas, which are among the largest recorded, and their versatility in structure and synthesis, allowing for a vast array of metal-ligand combinations and post-synthetic modifications. These features allow for the use of MOFs in several applications, including gas storage, catalysis, drug delivery, and contaminant removal. In addition, MOFs can be used during the sample preparation step in analytical applications. In fact, there are different microextraction techniques that have benefited from their use as adsorbents. In the case of in-tube solid-phase microextraction (IT-SPME), the MOFs is coated in the inner walls of a thin capillary. For the proper attachment of the MOF, different functionalization of the capillaries can be implemented [1].

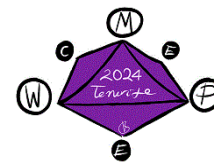
In this study, two strategies are proposed for the internal coating of fused silica capillaries with zirconium-based MOFs [2, 3]. The resulting devices were assessed in IT-SPME for their potential use in the determination of emerging pollutants, such as bisphenols and personal care products compounds.

Acknowledgments

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Preparation of metal-organic framework-coated blades by *in-situ* growth for analytical applications

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In the last years, metal-organic frameworks (MOFs) have shown attention due to their outstanding surface area, permanent porosity, and acceptable thermal and chemical stability. These materials consist of frameworks made of metallic centers connected through organic linkers, defining porous, and generally tridimensional structures [1].

Several analytical applications require the use of a thin layer of MOF supported on a flat surface like a stainless-steel sheet or a metallic mesh. When these thin film MOF devices are put in contact with aqueous media, they can adsorb compounds with high efficiency and in short extraction times in a procedure termed thin-film solid-phase microextraction (TF-SPME).

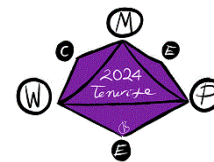
The main aim of this work is the development of a procedure for the preparation of MOF-coated blades based on stainless-steel blade and CIM-80(AI). The strategy implies mild functionalization of the blade support followed by the *in-situ* growth of the framework. The study also includes the characterization of the MOF-coated blades by powder X-ray diffraction and scanning electron microscopy and their use for the adsorption of polycyclic aromatic hydrocarbons from water.

Acknowledgements

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Activated carbons: a key material for closing the loop on resource use

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Population and waste generated have been growing in the last few years. In its interest, the circular economy is gaining interest because it tries to transform waste into other value-added products before they are dropped in landfills. Join with an increase in anthropogenic CO₂ emissions. According to the IPCC, the CO₂ emissions in 2019 were estimated at 59 tCO₂-eq, about a 12% increase from 2010 [1].

A reduction of this amount is indispensable for sustainable development. Currently, there are numerous studied technologies for CO₂ capture. Nevertheless, the production of adsorbents based on waste is a sustainable process. Activated carbons, carbon-based materials made from waste, are a promising adsorbent with low-cost production. They are produced in two steps: carbonisation and activation. The starting carbonisation step is pyrolysis, a thermal decomposition process in a non-oxygen atmosphere at temperatures between 300 and 700°C. Furthermore, from this process, char, bio-oil, and syngas are produced. Char produced is a solid porous material, which has improved physical properties in the second step. The second step is activation using activating agents such as CO₂, steam, or other chemical agents such as KOH, NaOH, and H₂SO₄. Pursuing the improvement of some parameters, such as surface, volume, pore size, or selectivity towards CO₂, the physical activation using a gaseous activator such as CO₂ or steam has a lower environmental impact than the chemical activation [2].

Activated carbons allow waste and CO₂ emissions reduction, two of the first key points for an ecological transition. In addition, bioenergy plays a key role in increasing the renewable energy rate because it is a manageable energy source, increasing the penetration of renewable energy compared to photovoltaic or wind energy. According to the IPCC, combining bioenergy production with CO₂ capture and storage accelerates the velocity to 2030 [1]. It can be produced from different resources as animal byproducts, biomass or organic wastes.

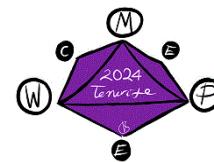
In conclusion, activated carbons play a pivotal role in closing the loop, minimising waste disposal in landfills, and effectively reducing emissions through their application as CO₂ adsorbents. The sustainability of this process stands as a critical factor in shaping a more promising and environmentally conscious future.

Acknowledgements

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Exploring more sustainable thermoelectric materials for enhanced energy harvesting from waste heat

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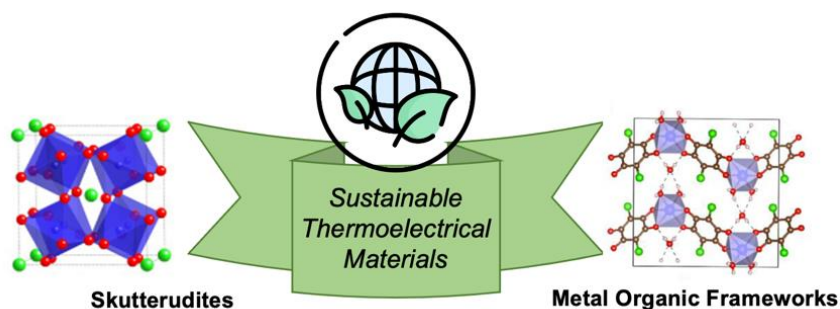
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Current commercial thermoelectric materials, primarily composed of tellurides, exhibit a modest energy conversion efficiency of about 6%. However, challenges such as the scarcity of elements, high toxicity, and limited applicability to specific temperature ranges hinder their widespread use. An essential goal is to address the constraints linked to traditional materials by exploring alternative compounds exhibiting enhanced thermoelectric properties.

Recent advancements have introduced new phases with higher energy conversion efficiency, with CoSb₃-based skutterudites showcasing improved thermoelectric properties, due to their isostructural nature with CoAs₃ minerals and the "Phonon-Glass Electron-Crystal" (PGEC) concept. Their structure, featuring large cavities, allows for the incorporation of diverse elements, acting as "rattlers" and reducing lattice thermal conductivity. As an alternative to cobalt minerals, Fe_{0.5}Ni_{0.5}Sb₃ represents a good starting point, given its shared isoelectronic and isostructural features with CoSb₃. [1, 2]

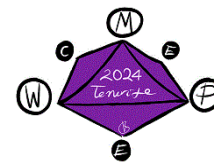
Metal-Organic Frameworks (MOFs) emerge as promising candidates for sustainable thermoelectric materials. Despite being recognized for their low thermal conductivity, MOFs have yet to be explored for thermoelectric applications. The project introduces a novel approach, employing MOFs with extended conjugation through ligands like dihydroxybenzoquinone (DHBQ) and chloranilic acid (CA) to enhance electrical conductivity. [3]

This comprehensive research of sustainable thermoelectric materials supports the global effort to establish more effective and eco-friendly energy systems by offering valuable insights for developing thermoelectric devices that can efficiently capture waste heat across a broader temperature range, promoting a more sustainable energy environment.



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Preparation of MXenes as catalysts for the oxygen reduction reaction

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The current environmental circumstances demand the development of alternatives to the use of fossil fuels as energy sources. To alleviate this issue, this work aims to synthesise new catalysts to replace noble metals used in energy conversion systems such as fuel cells. Two-dimensional (2D) materials have emerged as promising candidates for these devices, being transition metal carbides (TMCs) and nitrides (TMNs) the most used catalysts. These materials are generally obtained by selectively removing metal "A" from their precursor compound, called MAX phase, with the general formula $M_{n+1}AX_n$, where M is a transition metal, A represents an element mainly from groups 13 and 14, and X represents C or N, with $n = 1, 2, 3$ [1].

In this work, we developed a synthetic strategy to obtain MXenes. The materials were physiochemically (Raman spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM) combined with X-ray scattering spectroscopy (EDX)) and electrochemically characterised. Their electrocatalytic activity towards the oxygen reduction reaction (ORR) was studied in both acidic and alkaline media using cyclic and linear sweep voltammetry with rotating ring-disk electrode (RRDE) techniques.

Results confirmed that the synthesis of MXenes has been successfully developed. The catalytic activity observed for the ORR is low, so hybrid materials (with MOFs and MoS_2) were prepared to study the synergistic effect between them (Figure 1).

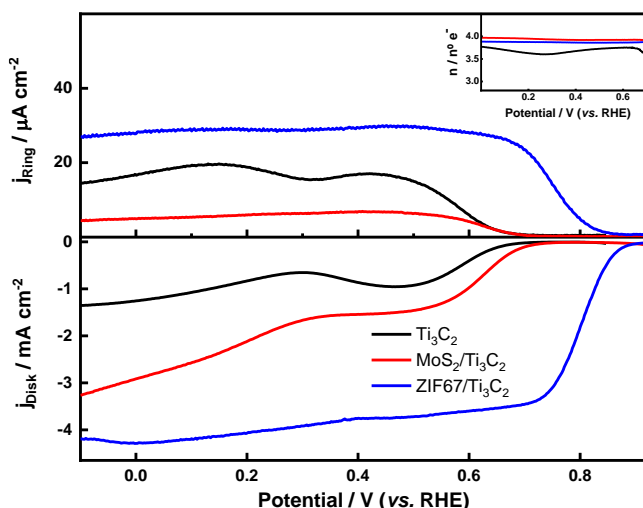


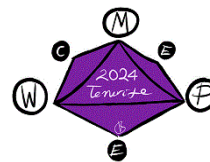
Figure 1. Anodic currents associated to H_2O_2 detection at the Pt ring during steady-state polarization curves for O_2 reduction at 1600 rpm in 0.1 M NaOH (top panels); cathodic currents recorded at the disk (bottom panels) and number of electrons transferred (n) (inset). Sweep rate of $0.002 V s^{-1}$.

Acknowledgements

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Chalcogenides supported on nickel foams as electrocatalysts for the hydrogen reduction reaction

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The environmental problems associated to the use of fossil fuels, such as the greenhouse effect, acid rains and holes in the ozone layer, could be avoided with the use of hydrogen as fuel [1]. Green hydrogen can be produced through water electrolysis, specifically in the cathode of electrolyzers, which usually are based on expensive noble metal catalysts [2]. Therefore, design of free-noble metals catalysts with high activity towards the hydrogen evolution reaction (HER) has capital importance to reduce the cost associated to this technology.

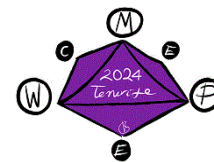
With the aim to suggest alternative materials to address HER with high performances, in this work, nickel chalcogenides have been synthesised on nickel foams and its electrocatalytic activity has been assessed. The catalysts were prepared by chemical etching of nickel foams in slightly acid media to form 2D structures with elevated content of OH groups, followed by sulfidation and selenisation processes. These materials were physicochemically characterised by X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS), confirming the formation of 2D structures and the correct incorporation of selenium and sulphur. Their electrochemical behaviour was evaluated by means of cyclic and linear sweep voltammetry, whereas precise determination of the HER onset potential and establishment of the rate determining step (rds) were achieved applying differential electrochemical mass spectrometry (DEMS). From these results it is concluded that 2D nickel chalcogenides can be suitable candidates for electrolyser cathodes.

Acknowledgements

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Plastic- and cellulose paper- based thin film membranes functionalized with ionic liquids for phenols remediation from water

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Ionic liquids (ILs) are solvents with melting temperatures below 100 °C and entirely composed by ions. Their main characteristics include great tunable capacity, negligible vapor pressure at room temperature, low flammability, modulable viscosity and solubility, and an impressive solvation capacity for a variety of compounds. Several subclasses of ILs have been developed in the last years. Among them, metal containing-ILs (MCILs) contain at least a metal component in their structure, whereas polymeric ionic liquids (PILs) are polymers prepared from an IL acting as monomer. Both MCILs and PILs possess some of the advantages of ILs, together with other features derived from their metallic and polymeric characters, respectively [1].

The use of ILs and PILs for the absorption of contaminants from water has been widely explored, whereas MCILs have been introduced more recently. ILs and derivatives can be directly used as solvents for the adsorption of contaminants or can be immobilized in membranes. This last option allows for using a large volume of IL or derivative, and the immobilization of the solvent onto the membrane facilitates its isolation after use [2].

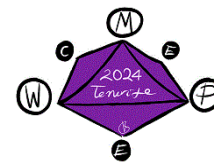
The objective of this work is to obtain membranes based on ILs, MCILs, and/or PILs supported on polystyrene, PTFE and/or cellulose paper. The preparation and characterization of materials and devices was performed, using different techniques, such as TGA, FT-IR. SEM and XPS images, etc. As proof of concept, the devices were applied for the elimination of phenols from water samples, in combination with high performance liquid chromatography and diode array detection.

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Merger of decatungstate photocatalysis and copper-catalyzed azide-alkyne cycloaddition reaction: an advanced strategy for the construction of 1,2,3-triazoles under green conditions

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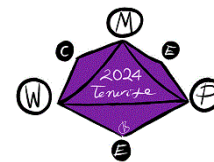
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1,2,3-triazoles are an important class of five-membered heterocyclic compounds present or used in various fields such as pharmaceutical, biological chemistry, and drug delivery research [1-3]. One of the commonly used strategies reported for the synthesis of 1,2,3-triazole compounds is copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) reaction, commonly known as the “click reaction” [4]. However, the major limitation of the CuAAC reaction is high copper and reducing agent loading, high temperature, long reaction time, and use of hazardous organic solvents. To advance more in this reaction, several strategies have been used to achieve an efficient, green, and sustainable protocols.

In this contribution, we report a dual catalytic system that has been successfully developed for the azide-alkyne ligation process to yield 1,4-disubstituted-1,2,3-triazoles. It consists of merging the decatungstate anion $[W_{10}O_{32}]^{4-}$ -photocatalyzed hydrogen atom transfer from ethanol as a source of hydrogen atom abstraction to produce the one-electron-reduced form $H^+[W_{10}O_{32}]^{5-}$, which reduces Cu(II) precursor into Cu(I) starting then the copper-catalyzed azide-alkyne cycloaddition reaction (CuAAC). The resulting bifunctional $H^+[W_{10}O_{32}]^{5-}/Cu$ catalytic system operates efficiently in an environmentally benign water–ethanol solvent mixture as reaction medium, resulting in the regioselective formation of 1,4-disubstituted-1,2,3-triazole derivatives, with high yields up to 99% and large substrate application scope under mild conditions. This dual catalytic approach has proven to function under sunlight exposition too with recovery and reuse of the catalytic system for several times [5].

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Study of the influence of the first transition metals on the enhancement of hydrogen production on P25 via water splitting

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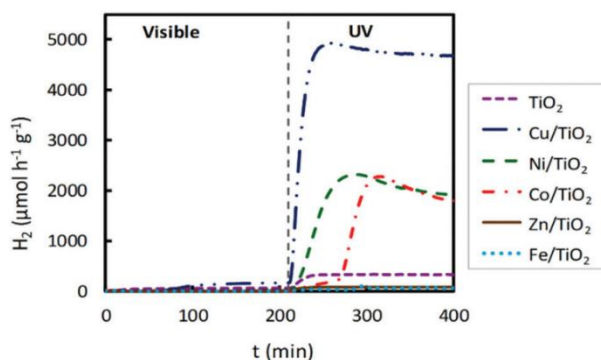
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In order to improve the photocatalytic response of TiO₂ to UV and visible light for hydrogen photoproduction [1], low cost M/TiO₂ semiconductor catalysts were prepared by the impregnation method of five different first row transition metals (M = Fe, Co, Ni, Cu or Zn) on a commercial titania support (Fig1). The maximum hydrogen production efficiency was achieved for the Cu/TiO₂ photocatalyst, with ~5000 and ~220 μmol h⁻¹ g⁻¹ H₂ production rates for UV and visible irradiation, respectively. The Cu atoms was highly dispersed over the TiO₂ support and the copper species existed as both reduced Cu⁰/Cu⁺ and oxidized Cu²⁺ on TiO₂. Besides, during the hydrogen production reaction, the reduced Cu was partially oxidized to Cu²⁺ by the transfer of photogenerated holes under UV or visible light irradiation [2]. With UV and visible lamps, the H₂

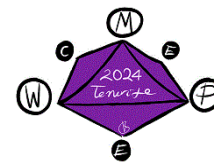


production rates were higher than those obtained with non-impregnated TiO₂ by factors of 16 and 3, respectively. These results demonstrated that a Cu/TiO₂ photocatalyst could be considered a promising low-cost alternative to the well-known Pt/TiO₂ system for hydrogen production, making the Cu-based catalyst an ideal cost-effective candidate for this reaction [3].

Fig 1. Hydrogen production is shown for the different transition metals.

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Multivariate metal-organic frameworks as adsorption materials in analytical applications

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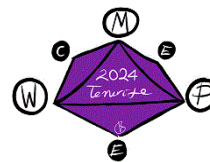
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Metal-organic frameworks (MOFs) are crystalline coordination polymers composed by a metal center (or metal cluster) coordinated by organic ligands. The geometry and structure of the crystal lattice vary depending on the selection of these secondary units. The MOF design process allows the creation of a wide variety of different materials. This heterogeneity does not end there. In fact, since 2010, more complex compounds called multivariate MOFs (MTV-MOFs) have been described. MTV-MOFs are formed by a metal center combined with two or more types of ligands. These materials allow for greater spatial structural diversity, as well as some heterogeneity, without altering the topology of the crystal. These changes seek a higher degree of functionality in the characteristics of the material, even improving the properties of the original structure. MOFs have been used for the extraction of analytes with interesting properties or with potential harmful effect on society (e.g. drugs, pollutants...) from environmental, biological, and food matrices samples.

In this study, Al(III) MTV-MOFs have been prepared using two different ligands, fumarate and mesaconate, which produce the well-known MIL-53(Al)-FA and CIM-80(Al) MOFs, respectively. The former has the structure of MIL-53 with rectangular pores, and it may exhibit a breathing phenomenon, while CIM-80(Al) has the MIL-68 structure with triangular and hexagonal pores. The objective of this work is the preparation of MTV-MOFs with different mesaconate:fumarate rates, and the evaluation of the ligand influence on the crystalline structure and the adsorption properties of the resulting MOF. The resulting materials were properly characterized, and the adsorption kinetics of the MOFs towards the extraction of different organic pollutants from water are also evaluated, thus gaining insights about the performance of this type of MOFs for their use in analytical applications.



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