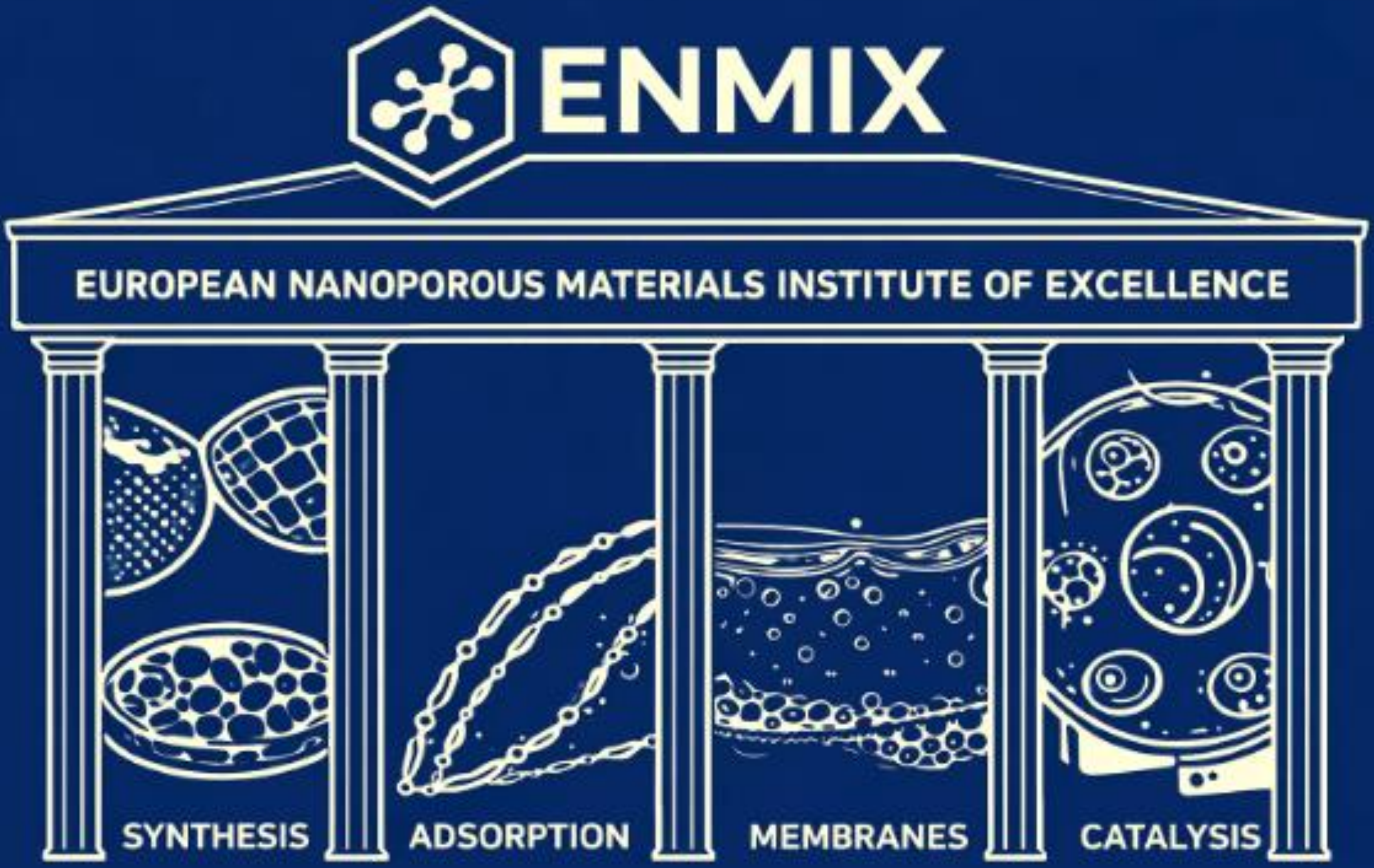
10th ENMIX WORKSHOP

Valencia, 16th & 17th April 2026



INSTITUTO DE
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QUÍMICA

Program overview

3rd floor "Cubo Azul" CPI from Polytechnic University of Valencia (UPV)

Thursday, 16th April 2026

8:30	**Registration**	
9:00	**Opening Session**	
9:30	**PL1**	**Avelino Corma**
10:30	O1	Deven P. Estes
10:45	O2	Inês Rodrigues
11:00	Coffee Break	
11:30	**IL1**	**Gregor Žerjav**
12:15	O3	José Luis del Río
12:30	O4	Natalia Malouchi
12:45	O5	Ana Rita Querido
13:00	O6	Niels Hansen
13:15	Lunch	
15:00	**IL2**	**Gianvito Vilé**
15:45	O7	Marta Mon
16:00	O8	Carola Vorndran
16:15	O9	Aljaž Škranjc
16:30	O10	Susana Valencia
16:45	**Poster Session + Snack**	

20:30	**Gala Dinner**

Friday, 17th April 2026

9:30	**PL2**	**Andrew M. Beale**
10:30	O11	Silvia Gutiérrez
10:45	O12	Ana Monteiro
11:00	Coffee Break	
11:30	O13	Nataša Novak
11:45	O14	Alejandro Serrano
12:00	O15	Eleni Iliopoulou
12:15	O16	Aymara Rodríguez
12:30	O17	Pablo del Campo
12:45	**IL3**	**Mercedes Boronat**
13:30	**Closing session**	
13:45	Lunch	

PL: Plenary Lecture (50'+10')
IL: Invited Lecture (35'+10')
O: Oral Communication (10' + 5')

Scientific Committe

- P. Cool (Univ. Antwerp)
- E. Iliopoulou (CPERI/CERTH)
- P. Oña-Burgos (ITQ)
- C. Martínez (ITQ)
- N. Novak Tušar (NIC)
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- P. Oña-Burgos (ITQ)
- J. L. Del Río-Rodríguez (ITQ)
- J. L. Cerrillo (ITQ)

PLENARY AND INVITED SPEAKERS

PLENARY SPEAKERS

Avelino CORMA
Institute of Chemical Technology
(Valencia, Spain)

Andrew M. BEALE
Research Complex at Harwell/UCL Chemistry/Methanox Ltd
(Harwell, England)

INVITED SPEAKERS

Gianvito VILÉ
Politecnico di Milano
(Milan, Italy)

Mercedes BORONAT
Institute of Chemical Technology
(Valencia, Spain)

Gregor ŽERJAV
Kemijski Inštitut
(Ljubljana, Slovenia)

Avelino CORMA - Design and synthesis of inorganic-microporous materials for gas separation and catalysis

Andrew M. BEALE - Identifying active sites for CH4 and CO2 conversion using operando spectroscopy

Gianvito VILÉ - Decoding the Structure and Enabling New Functions in Single-Atom Catalysts

Mercedes BORONAT - Mobility of Solvated Cu+ cations in Cu-Exchanged Zeolites Predicted By Machine Learning Accelerated Molecular Dynamics Simulations

Gregor ŽERJAV - Multifunctional plasmonic nanoporous photocatalysts for visible light and photothermal reactions

O1 - Improved Catalysis by Confinement of Organometallic Catalysts inside Mesoporous Supports

Wael Barakat,[1] Hoang-Huy Nguyen,[1] Erik Wimmer,[1] Zeki Beydeda,[1] Deven P. Estes[1,*]

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Homogeneous organometallic catalysts have many qualities (high activity per metal atom, high selectivity, low reaction temperatures, etc.) that could make them potentially attractive for many industrial applications. However, they suffer from severe drawbacks that limit their usefulness – especially catalyst instability and difficulty of separation from the reaction medium. One potential method for improving both the catalyst stability and the separability is to immobilize them on solid supports. This slows their deactivation by both stabilizing low-coordinate metal species by coordination to the surface and prevents bimolecular deactivation pathways due to the direct anchor to the surface. However, investigations have shown that often immobilized organometallic catalysts often show different catalytic behavior (activity, selectivity, etc.) from their homogeneous versions in solution. The reasons for this are however, up until now not particularly clear. The fact that the support plays a critical role in many catalytic reactions has been known in heterogeneous catalysis for quite some time. The reasons for these changes are often underexplored but include interesting effects such as changes in adsorption and diffusion of reactants, intermediates, and products, changes in the catalyst structure on certain supports, or even direct bond formation between supports and catalytically active species (e.g. strong metal-support interaction, SMSI). By using the lessons from heterogeneous catalytic studies, we can choose tailored supports for each catalytic reaction that give the desired reactivity increase instead of hindering the reactivity. We have applied this strategy toward the improvement of several different catalytic reactions including enyne cyclization reactions and CO_2 hydrogenation.

In the case of enyne cyclization reactions, we immobilized Pd complexes inside of carboxylic acid decorated SBA-15, which results in the protonation of the Pd to form an immobilized Pd-H species. We measured the equilibrium of the Pd-H formation via ^{31}P MAS NMR and found that the formation of Pd-H was less favorable in the pores than in solution.[1] This was due to lower acidity of the carboxylic acids confined in the pores than in homogeneous solution (by ca. 0.6 pK_a units).[2] Despite the lower amount of Pd-H in the pores, enyne cyclization was more efficient upon confinement in the pores (75% conversion vs. 12% conversion) because of 1) slower deactivation and 2) selective adsorption of the enyne reactant inside the pores leading to a high local concentration (as confirmed by MD simulations).

Amine-promoted CO_2 hydrogenation also works better on certain supports than in solution. We found that immobilization of a RuH_2 species onto ZnO gave a six-fold increase in turn-overs to the corresponding formamide product versus the homogeneous complex.[3] This is analogous to the improvement of heterogeneous CO_2 hydrogenation catalysts on Lewis acidic supports where the Lewis acid sites activate CO_2 towards hydrogenation and in this case toward formamide formation. We used this same effect to improve the reactivity of molecular Cu catalysts for CO_2 hydrogenation to MeOH. Immobilization of a phosphine-stabilized Cu-I complex onto various Lewis acidic supports activates the complex to MeOH formation (which is completely inactive in homogeneous solution). This effect is strongest inside of the Zr MOF NU-1000, which results in a 25x increase in the methanol activity at temperatures as low as 110 °C with greater than 95% selectivity (making no observed CO). This is due to the close contact between the Cu complex and the Zr nodes which activate both CO_2 and formate toward hydrogenation.

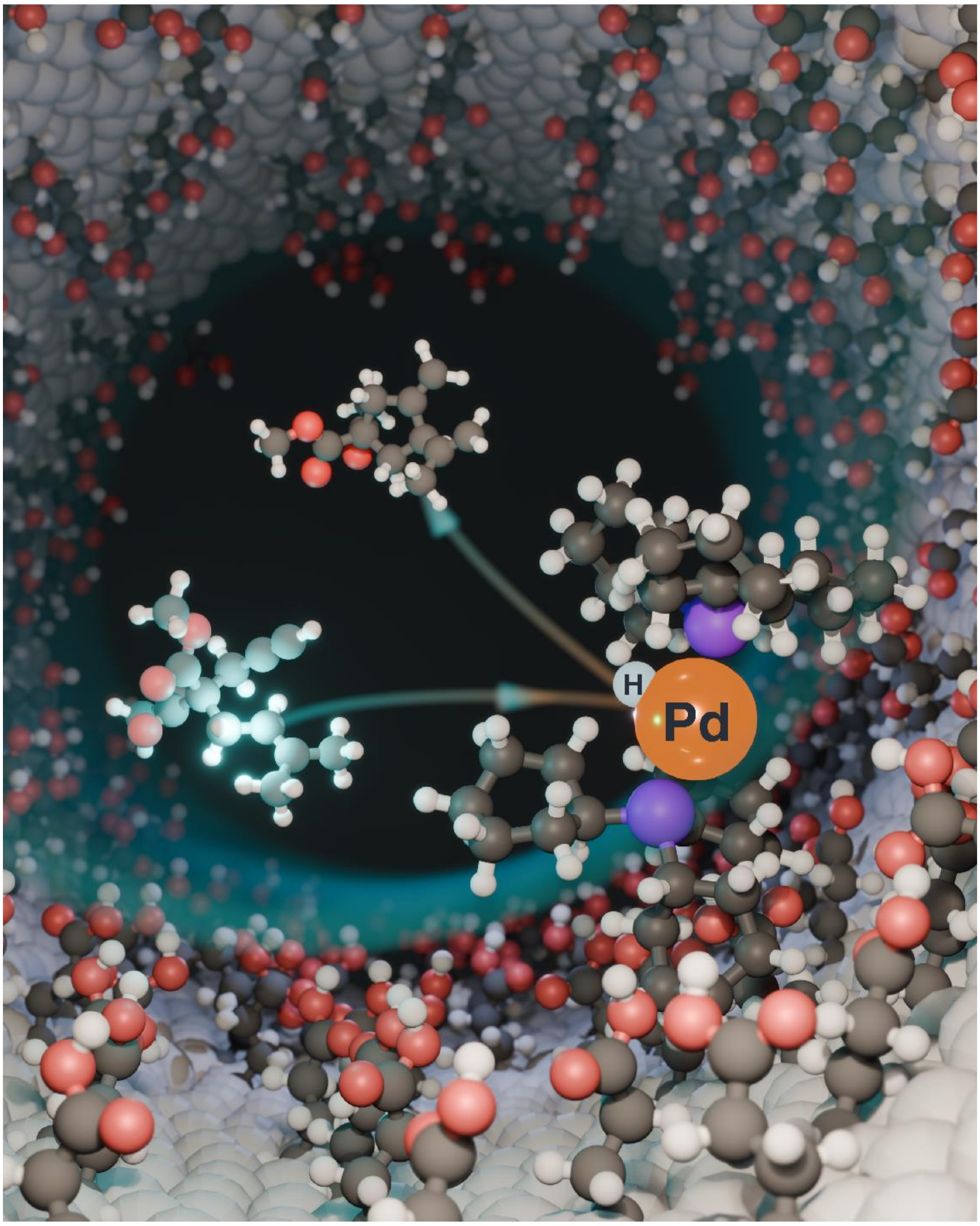

Fig.1. Artistic representation of the confinement of Pd-H in SBA-15 mesopores.

Funding

Deutsche Forschungsgemeinschaft (DFG Grant no. 358283783–SFB 1333/2)

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O2 - Development of MOR-40 Adsorbent for O_2/O_3 Gas Separation

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Ozone is a powerful oxidant commonly used in water treatment; however, ozone generators usually produce ozone concentrations below 15 wt.% [1]. To address this issue, O_2/O_3 gas separation using adsorption technology can concentrate the ozone stream while facilitating the recycling of the oxygen back into the generator. This study aims to develop an ozone-resistant adsorbent for separating oxygen and ozone.

Pellets were synthesized using zeolite MOR-40, colloidal silica, and water. The process involved mixing the binder with zeolite, extruding the paste, spheronizing the pellets, and calcinating them at 450 °C for 4 hours. The zeolite (in powder and pellet form) and the binder were characterized using N_2 adsorption at 77 K, CO_2 adsorption at 273 K, mercury intrusion porosimetry, helium pycnometry, X-ray diffraction, SEM/EDS analysis, and mechanical strength tests. Some results are shown in Table 1. The adsorption isotherms of O_2 were measured using a magnetic-suspension microbalance at 280, 303, and 323 K, under pressures up to 5 bar. The Langmuir model was fitted by minimizing the sum of residuals with a solver tool. Breakthrough curve experiments were performed in a lab-scale fixed-bed system, using a mixture of O_2 and O_3, with output measured by an ozone analyzer.

Table 1. Surface properties of MOR-40 samples and the binder

	Binder	**MOR-40 powder**	**MOR-40 pellets**	**Characterization method**
Surface area ($m^2\cdot g^{-1}$)	134.3 ± 0.1 (BET)	600 ± 1 (Langmuir)	557 ± 2 (Langmuir)	N_2 adsorption at 77 K
Micropore volume ($cm^3\cdot g^{-1}$)	-	$(1900 \pm 7) \times 10^{-4}$	$(1700 \pm 4) \times 10^{-4}$	N_2 adsorption at 77 K
Pore volume (<7.97 Å) ($cm^3\cdot g^{-1}$)	$(306 \pm 6) \times 10^{-4}$	$(2242 \pm 16) \times 10^{-4}$	$(1929 \pm 13) \times 10^{-4}$	CO_2 adsorption at 273 K
Skeleton density ($kg\cdot cm^3$)	2179 ± 2	2084 ± 5	2125 ± 3	He pycnometry
Apparent density ($kg\cdot cm^3$)	1364	589	1086	Hg porosimetry

The analysis of the results indicated a distinct selectivity for ozone adsorption, with ozone molecules being preferentially adsorbed over oxygen molecules. Moreover, tests revealed that the shaped material exhibits high resistance to ozone degradation, as evidenced by consistent and reproducible results across multiple trials. Therefore, the synthesized MOR-40 pellets can be used effectively for O_2/O_3 separation.

Funding

This work was supported by national funds by FCT/MCTES (PIDDAC) under OZONE4WATER, Project PTDC/EAM-AMB/4702/2020 (DOI: 10.54499/PTDC/EAM-AMB/4702/2020). This research was also supported by Fundação para a Ciência e a Tecnologia, I.P./MECI through national funds: LSRE-LCM, UID/50020/2025 (https://doi.org/10.54499/UID/50020/2025); and ALiCE, LA/P/0045/2020 (https://doi.org/10.54499/LA/P/0045/2020).

Acknowledgements

Inês Rodrigues acknowledges FCT for her PhD scholarship 2022.10784.BD.

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O3 - Alternating Magnetic Field-Assisted Electrocatalytic Oxygen Evolution Reaction in Encapsulated Co@C Nanoparticles

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Álvaro Gallo-Cordova,[3] M. Asunción Molina,[4,5] Jordan Santiago Martínez,[1]
Juan José Calvente,[2] Christian Cerezo-Navarrete,[1] Andrew M. Beale,[4,5]
María del Puerto Morales,[3] José Luis Olloqui-Sariego,[2] and Pascual-Oña Burgos[1]

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One of the main bottlenecks in producing hydrogen via water electrolysis is the intrinsically sluggish reaction rate of the oxygen evolution reaction (OER). In recent years, the application of an alternating magnetic field (AMF) to electrodes decorated with ferromagnetic metal nanoparticles has attracted increasing interest. Under AMF exposure, these nanoparticles can behave as self-heating, thermally activated electrocatalysts, providing localized heating that may accelerate reaction kinetics and, consequently, improve OER efficiency.[1]

In this study, we examine how both external operating conditions and the intrinsic properties of carbon-encapsulated, cobalt-based MOF-derived nanoparticles supported on graphite paper electrodes affect the coupled AMF-assisted OER process. In particular, we systematically evaluate the role of AMF amplitude, electrolyte composition (including concentration and the identity of the alkali cation) and cobalt loading in determining the overall electrocatalytic AMF-OER response.

The results demonstrate that applying an AMF leads to a pronounced increase in OER activity for **Co@C**-based electrodes, although the magnitude of this improvement depends strongly on the electrolyte formulation. Importantly, after prolonged and intense AMF-OER operation, the as-prepared catalyst preserves both its magnetic hyperthermia heating capability and its structural integrity. Detailed post-test characterization shows no evidence of sintering, cobalt leaching, or particle growth-degradation pathways that are commonly reported for metal nanoparticles subjected to strong magnetic fields. This confirms the remarkable operational robustness of the carbon-encapsulated cobalt catalyst under demanding conditions. Overall, these findings deepen the understanding of thermally driven AMF-assisted alkaline water oxidation and support the development of durable, high-performance catalysts for enhanced electrocatalysis.

Acknowledgements

J.L-R.R. wants to acknowledge MCIU for his PhD contract FPU21/2562. The authors want to acknowledge the Severo Ochoa Centre of Excellence program (CEX2021-001230-S).

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O4 - Layer-by-Layer Modified Ultrafiltration Membranes for Selective Removal of Hexavalent Chromium from Water

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The presence of hexavalent chromium (Cr(VI)) in natural and industrial waters is a major environmental concern due to its widespread occurrence and high toxicity. The parametric value for total chromium (including hexavalent chromium) in water intended for human consumption, according to Greek and European legislation (JMD D1(d)/GP 27829/2023 - Government Gazette 3525/B/2023) is set at 25 μg/L (effective from 2036). These regulations highlight the urgent need for efficient technologies capable of reducing Cr(VI) to very low concentrations. Conventional removal methods, such as reduction with ferrous iron, have significant limitations, including high chemical consumption, large sludge production, and the potential re-oxidation of Cr(III) to soluble Cr(VI) [1]. It is therefore important to develop suitable treatment technologies for the removal of Cr(VI) [2].

In this study, we investigate an alternative approach based on the modification of commercial ultrafiltration (UF) membranes using Layer-by-Layer (LbL) assembly. This technique involves the sequential deposition of cationic and anionic polyelectrolytes to form stable multilayer coatings with controlled surface charge, transforming conventional UF membranes from purely mechanical filters into materials capable of selectively binding anionic species such as chromate (CrO_4^{2-}) and dichromate ($Cr_2O_7^{2-}$). The modified membranes were characterized for surface morphology and composition, and their properties were compared with those of unmodified membranes. The results showed that the layer deposition process resulted in effective surface modification, as confirmed by scanning electron microscopy (SEM) combined with energy-dispersive spectroscopy (EDS), and Fourier transform infrared spectroscopy (FTIR). The effect of the multilayer structure on separation performance was evaluated under different pH conditions, confirming the role of electrostatic interactions in Cr(VI) retention. Removal experiments demonstrated a significant improvement over unmodified membranes, effectively reducing Cr(VI) concentrations to levels consistent with current regulatory standards.

These findings demonstrate the potential of LbL-modified UF membranes as a sustainable and energy-efficient solution for the direct removal of Cr(VI) from water. Building on laboratory-scale optimization, a pilot-scale treatment unit has been constructed to evaluate membrane performance and operational stability under realistic conditions, demonstrating the technology’s readiness for application in drinking water treatment.

Funding

This research is co-financed by the European Union and Greek national funds through the Operational Programme “Human Resources Development, Education and Lifelong Learning,” under the call “Partnerships of Excellence in Research and Innovation-SUB1.1” (Action Code: 16289, project acronym: Smart-Mem-Mat).

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O5 - Engineering $CN^{o}T$–CeO_2 Composite Supports for CuZn Catalysts in CO_2-to-Methanol Conversion

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CO_2 emissions have continuously increased in recent years due to the combustion of fossil fuels for energy production, contributing to the aggravation of climate changes [1]. To mitigate these emissions, CO_2 hydrogenation to methanol, a concept proposed by George Olah as “methanol economy”, has become one of the most researched approaches, because it promotes the conversion of CO_2 to a value-added product [2, 3]. Nevertheless, the search for more efficient catalysts remains ongoing, as the commercial catalyst, $Cu/ZnO/Al_2O_3$, suffers deactivation under industrial operating conditions [3]. Innovative supports of composites of carbon nanotubes (CNT) and Cerium Oxide (CeO_2) will be developed to further enhance catalytic performance and reduce the use of rare and expensive metal oxides.

Bimetallic catalysts comprising copper (Cu) and zinc (Zn) nanoparticles supported on composites of commercial or functionalized CNT and CeO_2 were developed. The supports were prepared using various methodologies to assess the influence of the preparation method - ball-milling, precipitation or incipient wetness impregnation - and CeO_2 source - precipitated or commercial - on catalytic performance. Furthermore, a thermal treatment with 5% of H_2 was performed on the supports prepared by ball-milling and precipitation, to evaluate if more oxygen vacancies can be formed and thus, improve CO_2 adsorption. The catalytic experiments were conducted between 150 and 300 °C, and 30 bar (GHSV = 7 200 $cm^3\ g^{-1}\ h^{-1}$) in a Microactivity Reference reactor from PID Eng & Tech. The permanent gases were analysed with a DANI GC 1000, with a TCD, and methanol was examined using a DANI GC 1000, with a FID detector. The catalysts were extensively characterized by various techniques.

At 250 °C, all catalysts were active and exhibited higher selectivity towards methanol than CO. Functionalized CNT did not improve catalytic performance compared to the catalyst supported on the composite with pristine CNT. Nevertheless, in both cases where an H_2 thermal treatment was performed, $CuZn/CNT\text{-}CeO_{2\ P\ 5\%\ H_2}$ and $CuZn/(CNT\text{-}CeO_2)_{P\ 5\%\ H_2}$, an improvement in CO_2 conversion was observed compared to the catalysts that did not undergo H_2 thermal treatment. Among all catalysts evaluated, $CuZn/CNT\text{-}CeO_{2\ P\ 5\%\ H_2}$ achieved the highest methanol yield. A long time-on-stream (TOS) experiment was performed with this catalyst, which remained active for 100 h at 250 °C and 30 bar.

Acknowledgements

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O6 - Leveraging classical density functional theory and molecular simulations to study properties of fluids confined in micro- and mesoporous materials

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Understanding the distribution and mobility of molecules in confinement is a prerequisite to utilize confinement effects in the realm of molecular heterogenous catalysis, liquid chromatography, or gas adsorption. Molecular simulation studies offer spatiotemporal resolution for confined systems that is often not accessible experimentally. Crystalline porous materials such as zeolites or metal-organic frameworks offer great potential in gas adsorption, separation, and storage. The vast design space requires efficient computational approaches that allow for screening approaches. Molecular simulations are often not suitable for this purpose. Classical density functional theory offers an efficient alternative for adsorbates with modest polarity, reducing computational costs by up to three orders of magnitude, compared to molecular simulations [1]. To study confinement effects in ordered mesoporous materials such as functionalized silica, structural models are required that replicate the geometry, dimensions, and chemical structure of a surface-functionalised porous material. We present a software tool that facilitates rapid model building of functionalised silica pores for systematic studies of confinement effects in various applications of relevant materials using molecular simulation [2]. We illustrate how the tool can be used to study a diverse set of research questions arising in experimental studies of molecular heterogenous catalysis in confined geometries. These examples encompass the phase behavior of solvent mixtures under confinement, the distribution of reactants and products in mesoporous silica, and the benefit of confinement to focus the conformational space accessible to a catalytic complex.

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O7 - MOFs and zeolites as catalysts for carbenoid reactions

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Nanoporous materials provide a unique platform to modulate catalytic reactivity through site isolation, confinement effects, and precise control of active center environments. In this contribution, we present the evolution of our catalytic systems for carbenoid transformations from a materials-design perspective, highlighting how framework architecture governs the generation and stabilization of active species.

Our work initially focused on the preparation of a quasi-linear Pd_4 cluster stabilized within a crystalline Metal–Organic Framework (MOF) [1]. This material represents one of the earliest examples of a well-defined supported metal cluster capable of catalyzing challenging carbene-mediated reactions, such as the Büchner ring expansion reaction. This concept was subsequently extended to ultrasmall Ag clusters confined within porous matrices, including MOFs and zeolites, where metal nuclearity and metal–support interactions were found to critically influence activity and selectivity [2,3]. A major advance was achieved with the discovery that a dealuminated zeolite Y, entirely metal-free, efficiently promotes these transformations [4]. Detailed catalytic and structural analysis indicates that confined Brønsted acid sites within the microporous framework are sufficient to stabilize reactive carbene intermediates and enable selective insertion reactions under mild conditions. This finding challenges the long-standing assumption that metals are indispensable for carbene chemistry and reveals the catalytic potential of zeolite acidity combined with confinement.

Overall, these results illustrate how deliberate engineering of pore topology, acidity and site isolation enables the transition from supported metal clusters to metal-free zeolitic catalysts (Fig.1.), opening new opportunities for sustainable catalytic design [5].

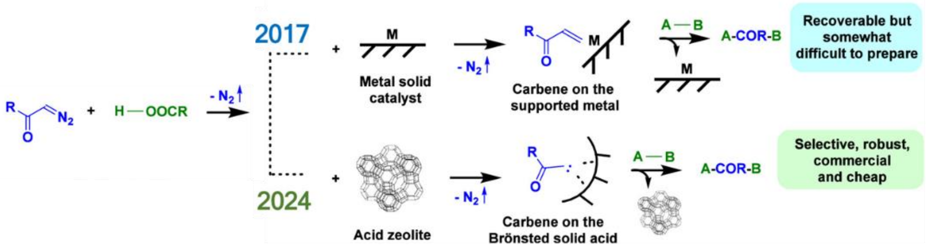

Fig.1. Conceptual evolution of solid catalysts developed for carbenoid reactions in our research journey, highlighting the transition from supported metal catalysts to confined Brønsted acid sites in metal-free zeolites.

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O8 - Advanced Wettability Characterization of Zeolites and Silica by Combining Adsorption with NMR Relaxometry

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The wettability of nanoporous materials plays an important role for their application, e.g., in separation and catalysis, since tuning the wettability can enhance the affinity and selectivity of certain compounds. Hence, a detailed investigation of the relation between structural properties, wettability and the resulting process performance is necessary. Within this context, we have recently shown that NMR relaxometry can be applied for surface area assessment of nanoporous materials immersed in a liquid phase [1] but also shows potential for pore size analysis [2]. This study focuses on wettability characterization of nanoporous materials.

The assessment of the wetting behavior of fluids inside of pores is challenging and usually requires a combination of different experimental tools. Within this context, we demonstrate that NMR relaxometry is a valuable complementary tool for fast wettability characterization. In fact, it had been demonstrated that, the ratio of the spin-lattice to spin-spin relaxation time (T1/T2) is correlated with effective attractive interactions of fluid molecules with surfaces, i.e. including with pore walls [3] and hence contains information about the wetting behavior of an adsorbate. However, this ratio can also be affected by textural properties. To address this limitation, this study suggests a novel methodology for wettability quantification based on the spin-lattice to spin-spin relaxation time ratio of the adsorbed liquid film on the pore surface (T1,ads.film/T2,ads.film-ratio), calculated based on the ratio of spin-lattice and spin-spin surface relaxivities [4]. This novel approach allows for the determination of a characteristic value, solely affected by the wettability. This is demonstrated using a series of zeolites with different silicon-to-aluminum ratio. The study shows, for the first time, a correlation between the T1,ads.film/T2,ads.film-ratio of water in contact to zeolite and the hydrophilicity index determined from water vapor adsorption experiments. In addition, the applicability of the T1,ads.film/T2,ads.film-ratio for fast wettability quantification is shown for mesoporous silica functionalized with different hydrophilic and hydrophobic surface functional groups in comparison to the contact angle of the adsorbed water film determined with water vapor adsorption and water intrusion experiments.

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O9 - Mechanochemical solvent screening towards a green synthesis of ZIF-94 with closed loop solvent recycling

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Zeolitic imidazolate frameworks (ZIFs), a subgroup of metal-organic frameworks (MOFs), have in recent years been extensively studied for sorption applications due to their superior stability and kinetics for vapour/gas adsorption if compared to some carboxylate-based MOFs. The ZIF-94 (also known as SIM-1) with SOD topology is a broadly studied ZIF with potential uses in CO_2 capture [1], (2.2 mmol @25°C 1bar) and CO2/N2 separation [2] when used as part of Mixed Matrix Membranes. One of the problems with utilizing some ZIFs, including ZIF-94, in sorption and separation applications is that the metal coordination flexibility and particular linker and metal combinations lead to the coappearance of multiple stable phases with different topologies.

Initially, mechanochemistry was used for solvent screening due to its short synthesis times. This included water and various alcohols (methanol to butanol). In the case of water and methanol, after milling and aging of the sample for a day, we observed only the RHO phase of ZIF-93. Prolonged aging without washing led to the slow formation of a mixed phase system.

We successfully prepared ZIF-94 both mechanochemically and solvothermally using only ethanol and water as solvents. The synergistic use of ethanol's structure directing role and water as a kinetic modifier allowed for preparation of well crystalline phase pure ZIF-94 with clearly defined cubic particles. The use of ethanol/water instead of THF allows for easier activation of the resulting ZIF, reducing the required solvent needed for washing and solvent-exchange, making the synthesis ever greener. The developed solvothermal method allowed for semi-closed loop solvent recycling, where the bulk of the solvent could be easily reused without purification steps required. Only the solvent adsorbed in the product had to be compensated for in the recycling. After 5 reuses, no significant change in sorption or morphology was observed in the final product.

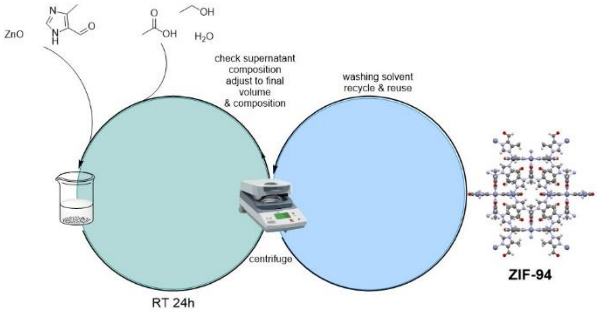

Fig.1. Proposed loop system for cycling reuse of solvent

Funding

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O10 - Revealing the Potential of Siliceous Zeolites for Separation Processes

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Many gas and vapour separation processes require complex infrastructures and/or are very energy-intensive, making the search for more sustainable alternatives highly desirable. Examples of such separations include CO_2 adsorption for natural gas and biogas upgrading, separation of light olefins and recovery of bioalcohols from fermentation broths, among others [1]. These separations are highly challenging and entail an enormous economic impact, since current technologies that involve cryogenic distillation, amine scrubbing or extraction-evaporation-distillation processes could be replaced by less energy consuming separation units based on the use of porous materials as selective adsorbents [2].

Among porous materials, zeolites arise as excellent candidates due to their particular properties, such as the uniform porosity in the range of the size of the molecules to be separated, the high stability and robustness. In fact, zeolites are utilized as selective adsorbents in several separation processes, as desiccants, in N_2/O_2 separation, in H_2 purification or in linear from branched hydrocarbons separation, among others [3]. The main properties of zeolites that influence their behaviour as selective adsorbents are the pore aperture and topology and the chemical composition, which can be varied from Si/Al ratio of 1 to purely siliceous composition. In this way, polarity, acidity and hydrophobicity can be modified adequately to tune the interaction with the molecules to be adsorbed in the separation process.

In this context, the applicability of zeolites with pure silica composition in different separations is the objective of this work. One of these processes involves olefins separation and the advantage of pure silica zeolites as adsorbents relies on the complete absence of acid sites that prevents pore blocking caused by olefin oligomerization within the porosity. It will be shown how subtle modifications in pore opening can have a significant effect on the selectivity during competitive adsorption and the influence of zeolite framework flexibility in the adsorption behaviour [4]. Medium-pore pure silica zeolites will also be presented as selective adsorbents to separate linear and mono-branched from multi-branched alkanes in the gasoline range with the objective of the enrichment of the streams in branched components to increase its octane number [5].

Other separations in which pure silica zeolites have shown great promise are vapour phase adsorption recovery processes to isolate bioalcohols in mixtures obtained from fermentation media in which the alcohols are diluted in water in very low concentrations. In these cases, the hydrophobicity of pure silica zeolites becomes a key parameter to maximize alcohol recovery [6,7,8].

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O11 - Green One-Pot Synthesis of Benzimidazoles in Water Using a Ru-Doped Co-Based Heterogeneous Catalyst

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Benzimidazoles are highly valuable nitrogen-containing heterocycles widely present in pharmaceuticals and agrochemicals [1]. Classical synthetic methodologies usually involve multistep procedures, acid promoters and non-sustainable solvents, leading to poor atom economy and waste generation [2,3]. In this contribution, we report a green one-pot strategy for the hydrogenative coupling of 1,2-dinitroarenes with aldehydes in water, employing molecular hydrogen as a clean reducing agent.

A novel Ru-doped cobalt catalyst (Co–Ru@C) was synthesized by pyrolysis of a Ru-incorporated Co-based metal–organic framework supported on carbon. The material contains ca. 10 wt% Co and only 1 wt% Ru, minimizing noble metal usage while significantly enhancing catalytic performance. In situ PXRD and XAS studies confirmed the reduction of both metals during pyrolysis and revealed interfacial Ru–Co interactions. HAADF-STEM analysis showed cobalt nanoparticles (~18 nm) surrounded by small Ru nanoparticles (~2 nm), supporting a synergistic catalytic interface.

Under optimized conditions (135 °C, 15 bar H_2), Co–Ru@C achieved quantitative conversion and >99% selectivity toward 2-phenylbenzimidazole in water, clearly outperforming the monometallic Co@C analogue. This catalyst exhibited excellent recyclability over five consecutive cycles and is active for the obtention of more than 20 substituted benzimidazoles in high yields.

Overall, this work demonstrates how minimal noble-metal doping in MOF-derived heterogeneous catalysts enables efficient, scalable and environmentally benign cascade hydrogenations in water [4].

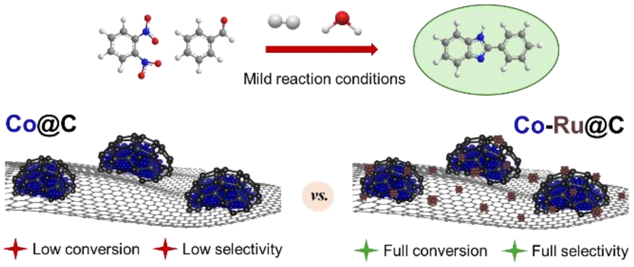

Figure 1. Greener one-pot benzimidazole synthesis from dinitroarenes achieves complete conversion and selectivity with a Ru-doped Co catalyst in water using hydrogen.

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O12 - CO_2 capture from humid gas streams with MOF based hybrid materials by Electric Swing Adsorption (ESA)

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Carbon dioxide (CO_2) is the primary greenhouse gas responsible for climate change, which is largely driven by human activities.[1] According to assessments by the Intergovernmental Panel on Climate Change (IPCC) and the International Energy Agency (IEA), carbon capture, utilisation, and storage (CCUS) will play a crucial role in reaching “Net Zero” emissions by 2050.[2,3] Although solvent-based absorption remains the most commonly employed CO_2/carbon capture technology, the use of solid adsorption methods is steadily increasing. The efficiency of the adsorption process depends critically on the choice of adsorbent, the regeneration method, and the duration of the adsorption cycle. [4] Electric Swing Adsorption (ESA) is an emerging technology with great potential as a regeneration method and has attracted great attention from governments, industry and academia in recent years. In this work an extensive literature review was performed related to highly capable adsorbents for CO_2 capture using Electric Swing Adsorption (ESA) with the aim to create an adsorber for CO_2 capture from streams with methane, nitrogen, and water. The selected materials were ZIF-8, Al-Fum, UiO-66, Zeolite 13X, MOF-74(Ni), and Cu-BTC. Hybrid materials with electrification capability were prepared by combining two carbon-based materials (activated carbon and graphite) with the six selected adsorbents. The hybrid materials were prepared by extrusion followed by pelletization. From this process resulted twelve distinct formulations, each consisting of 45 wt.% adsorbent, 45 wt.% activated carbon (AC) or graphite, and 10 wt.% carboxymethyl cellulose binder. All hybrid materials were characterized by N_2 adsorption at 77 K, CO_2 adsorption at 273 K, helium pycnometry, mercury intrusion porosimetry, sweeping electron microscopy and energy dispersive spectroscopy. The CO_2, CH_4, N_2 and H_2O equilibrium adsorption isotherms at 30 °C were measured for all hybrid materials. Preliminary electrification tests were conducted using a small packed bed, with copper electrodes and an electrical source to simulate the column electrification. The results obtained for a voltage of 40 V, showed some graphite hybrid materials achieved higher temperatures faster, approaching 100 °C.

Table 2: Physical characterization of the 4 hybrid materials with highest CO_2 adsorption.

	MOF-74(Ni)_AC	13X_AC	MOF-74(Ni)_Graph	13X_Graph
BET surface area (m^2/g)	1941	1782	341	140
Volume of micropores (cm^3/g)	0.35	0.27	0.24	0.13
CO_2 adsorbed @ 303 K, 1 bar (mol/kg)	2.991	2.639	2.048	1.598

Funding

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O13 - Potential of Functionalized Nanoporous Silicates for Fenton-like Catalytic/Photocatalytic Water Cleaning

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Organic compounds are the main class of wastewater pollutants emitted from various industrial processes. Advanced oxidation processes (AOPs) are one of the most efficient chemical methods for removal of organic compounds from wastewater. Recently, different systems of advanced oxidation processes (AOPs) as chemical methods have been intensively investigated because they can totally decompose organic pollutants to inorganic compounds such as H_2O, CO_2 and inorganic species. Most of AOPs use a combination of strong oxidizing agents (e.g. H_2O_2, O_2, O_3) with catalysts (e.g. transition metals or transition metal oxides) and/or irradiation (e.g. UV and visible light). AOPs main function is the generation of highly reactive free hydroxyl radicals. Hydroxyl radicals can totally destroy organic pollutants soluble in water or convert them into more biodegradable compounds as a pre-treatment stage. The AOPs bottleneck is high cost of the catalysts. The way to improve the cost-efficiency of AOP systems is to develop of more efficient but low-cost catalysts that would contribute in satisfying environmental regulations.

Transition metals or transition metal oxides immobilised on a silica porous supports are an example of low-cost catalysts or photocatalysts suitable for AOP. The nature of the support and the method of immobilisation of catalytic species are critical as the surface area and functionality determine the nature and dispersion of the metal or metal oxide nanoparticles and hence their catalytic activity. We have recently evaluated the catalytic/photocatalytic efficiency of bimetal silica supported Fenton-like AOP catalysts. An overview on the potential of these nanoporous materials will be presented.

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O14 - Counterbalancing cation control of the hydroformylation reaction catalyzed by subnanometer Rh–supported FAU zeolites

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The hydroformylation of alkenes is among the multi–ton reactions in industry still performed with soluble and expensive Rh metal catalysts.[1] Consedering the proven efficiency of zeolites in industrial processes, together with the inertness of aluminosilicate framework towards *syn* gas and the ease of incorporating Rh species into the zeolite structure, Rh–supported zeolites have emerged as leading potential candidates for the solid–catalyzed hydroformylation of alkenes, with extensive studies reported during over recent years. [2,3]

In this work, we demostrated that the counterbalancing cations of the zeolite, inherent to these aluminosilicates, significantly impacts on the catalytic activity and selectivity of the hydroformylation reaction.[4] We show here the synthesis of ligand–free, ultrasmall Rh^{1+}–oxide species in FAU zeolites with different counterbalancing cations by impregnation-calcination methods. The Rh active sites catalyze the hydroformylation reaction of alkenes as a function of the counterbalancing cation, not only in terms of overall catalytic activity (conversion) but also with respect to selectivity toward aldehyde products, thus providing a structure–activity reliationship for this reaction. The ligand–free Rh–zeolites can now be rationally selected for different alkene reactants and can also be used to perform one–pot hydroformylation/acid-catalyzed reactions, thereby opening new ways for the design of solid catalysts for these paramount reactions.

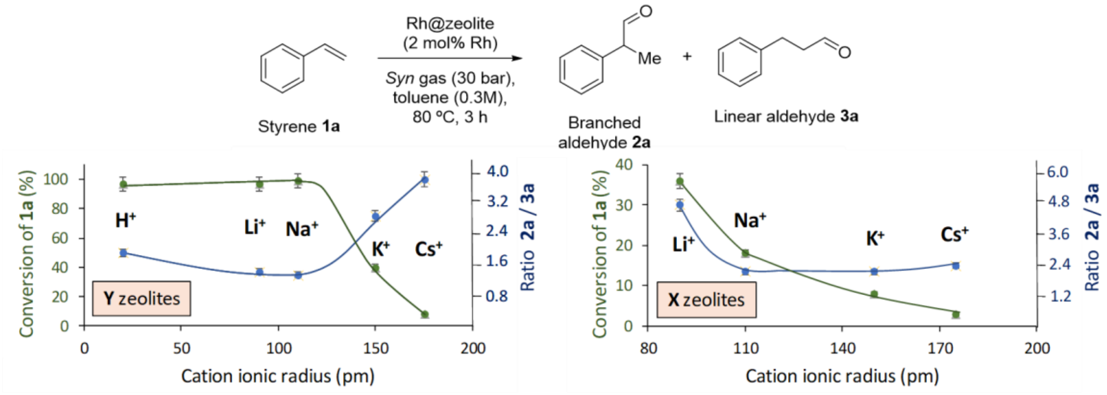

Fig. 1. Catalytic results for the hydroformylation reaction of styrene with different Rh–zeolites under the indicated reaction conditions (syn gas = 45% CO + 45% H_2 + 10% Ar).

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O15 - CO Preferential Oxidation over Co/alumina Catalysts

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Developing technologies for the efficient removal of trace CO from hydrogen is critical to protect the Pt anode from poisoning and ensure the stable operation of Proton exchange membrane fuel cells (PEMFCs). Among conventional approaches for CO elimination from hydrogen-rich gas mixtures CO-PROX represents the most mature and efficient alternative due to its simplicity, outstanding efficiency to maintain CO concentrations below 10 ppm, its practicality and its cost-effectiveness. The development of highly efficient CO-PROX catalysts is crucial, with active metal selection primarily focusing on precious metals (e.g., Au, Pt, Ru) and non-precious varieties (e.g., Co, Cu, Mn) [1, 2]. Due to high cost and thus constrained application of noble metal-based catalysts, research attention has shifted towards transition metals. Currently, a large number of studies focus on transition metal oxide catalysts such as cobalt (Co_3O_4), copper (CuO, Cu_2O), manganese (MnO_2, Mn_2O_3, Mn_3O_4) and iron oxides (Fe_2O_3, Fe_3O_4) [2,3]. Among these, cobalt oxide materials are inexpensive and exhibit excellent redox properties, making them one of the most effective catalysts for CO-PROX reaction [4].

In the present work, a series of catalysts based on alumina and impregnated with Co or Fe (1, 5% wt.) were prepared and thoroughly characterized. Either wet or spray impregnation method were used for the synthesis of cobalt and iron-based materials. The dry impregnation method was also used to incorporate palladium (0.5% wt.) on the Co/γ-Al_2O_3. The physicochemical properties of all catalytic materials were studied, focusing on the surface area (BET method) and on the identification of the formed metal phases with XRD method, present both in fresh and used catalysts (after reaction). The catalysts were evaluated for the selective oxidation reaction of CO (PROX-CO), using a gas feed composition of: 0.5% vol. CO, 0.5% vol. O_2, 40% vol. H_2 and He. Both the effect of the metal and the synthesis method were investigated. The results revealed cobalt as a more effective transition metal than iron, while the 5% wt. Co/γ-Al_2O_3 prepared by the spray-impregnation method (5Co/Al-SI) presented the optimum CO-PROX performance, probably due to the deposition of the formed Co_3O_4 (as identified by XRD method) on the outer surface of alumina, creating a core-shell nanostructure, according to the morphological characterization (SEM method). Promotion with Pd did not favor the reaction at high temperatures, while the opposite was observed at low temperatures.

The catalyst 5Co/Al-SI was further explored to investigate the effect of space velocity (WHSV) and H_2 content in the feed mixture. The stability of the optimum catalyst was also studied over 16 h of reaction, at constant temperature (T: 280°C) and a decrease in the CO conversion (from 74% to 44%) was observed after 16 h of reaction. Water presence (10% vol.) in the feed decreased the catalytic performance, while subsequent water removal revealed encouraging results, as it partially restored the catalytic activity. The characterization of the used catalysts proved that their surface properties did not significantly change, while differences were observed in the cobalt oxidation state, as in the XRD diffractograms the intensity of the Co_3O_4 peaks were decreased and a peak due to CoO appeared.

Finally, the Co metal loading was further increased (10% wt.) resulting in enhanced CO-PROx performance especially after a reductive treatment. Bimetallic configurations (Fe-Co) were also explored, leading to promising results. As metal oxidation state is crucial for the PROx reaction, selective reduction with ascorbic acid was further investigated.

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O16 - Design Of Co/N-Doped Carbon Catalysts for CO_2 Conversion Via Reverse Water-Gas Shift (RWGS).

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The continuous increase in atmospheric CO_2 emissions has intensified the development of catalytic technologies capable of converting CO_2 into value-added chemicals while reducing environmental impact [1]. Among the available approaches, the reverse water–gas shift (RWGS) reaction offers a viable pathway to produce CO as a key platform molecule. However, its endothermic nature typically requires high operating temperatures (>600 °C), highlighting the need for highly efficient catalysts active at lower temperatures [2]. In this context, metal single-atom catalysts (SACs) have emerged as promising candidates due to their maximum atom utilization, fully exposed active sites, and enhanced activity, stability, and selectivity [3].

In this study, the synthesis of cobalt-based catalysts supported on N-doped carbon ***(Co@NC1-9)*** was optimized to promote CO production through the RWGS reaction at a low temperature. For that, a Taguchi L9 experimental design was employed to evaluate the influence of cobalt loading (2, 5, and 10 wt.%), sonication time (15, 30, and 60 min), and first and second calcination temperatures (150–350 °C and 450–650 °C, respectively). A ***NC (MelCit 2:1 P850)*** was selected as a support due to its physicochemical and structural properties [4]. The catalytic activity was evaluated a temperature range of 450–600 °C, using 50 mg of catalyst and a H_2: CO_2/He (4:1) gas mixture, at a continuous flow rate of 100 mL/min.

Characterization by transmission electron microscopy revealed porous carbon structures with a good distribution of cobalt nanoparticles of different sizes. Particle sintering and growth increased with higher second calcination temperatures, whereas longer sonication times improved dispersion. Moderate calcination temperatures yielded controlled particle sizes and narrow distributions. Notably, ***Co@NC9*** exhibited the highest metal dispersion and the smallest particle size (~1–2 nm), with no diffraction peaks detected by XRD, indicating highly dispersed cobalt species below the detection limit. Catalytic tests showed the expected increase in CO_2 conversion with temperature, consistent with the endothermic nature of RWGS, together with high selectivity toward CO. ***Co@NC9*** demonstrated the best performance, reaching ~70% CO_2 conversion at 600 ºC, and maintaining significant activity at lower temperatures. This behavior is attributed to the excellent dispersion of cobalt and strong anchoring at Co–Nx sites promoted by nitrogen doping, likely involving small clusters or isolated single atoms. Overall, the scalable two-step annealing method enables effective metal dispersion, removes weakly interacting species, and suppresses sintering. The experimental design successfully identified optimal preparation conditions to minimize particle size and maximize metal dispersion, resulting in highly active Co-based catalysts for low-temperature RWGS applications.

Funding

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O17 - Extending the design of ZSM-5 zeolite as catalyst for the butene-to-propylene reaction. Impact of the crystal morphology

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The beneficial use of zeolites as shape-selective catalysts has been widely demonstrated for petrochemical and refine processes. They can be considered as nanoporous reactors since they allow transformations of molecules inside their well-defined system of micro- and nano-sized channels and cavities, which ultimately governs activity, selectivity and catalyst life-time. The design of the zeolite properties from the synthesis is crucial for their successful use. It is well documented that the intrinsic pore dimensions and shape, chemical composition (Si/Al ratio) and crystallite size (pore length) determine the number and distribution of the active sites as well as the diffusion pattern. Taking a further step, we have included in this work the crystal morphology as a fundamental descriptor. In particular, we show how the direction of the pores running along the different crystallographic dimensions and the preferential exposure of certain crystal facets impact the shape-selective and diffusion properties.

In this study, a series of ZSM-5-based catalysts were prepared for maximizing the propylene production by oligomerization-cracking of butene,[1] which constitutes an inexpensive on-purpose process to alleviate the demands of propylene as well as to exploit the butene stream co-produced by the high-volume FCC technology. ZSM-5 zeolite is an excellent candidate for performing this reaction. It is composed of intersecting medium pore-sized pores with straight or sinusoidal architecture that offer a good compromise between catalyst life and propylene selectivity. Nevertheless, the extent of the space created at the channel intersections and the length of the straight pores should be minimized, since they involve consecutive reactions (re-cracking) and promote the formation and/or diffusion of (poly)alkylated aromatic molecules,[2,3] which lead to lower propylene selectivity and faster catalyst decay.

We have defined chemical composition, crystal size and crystal morphology as the three descriptors that should control activity, selectivity and catalyst life. Then, we have synthesized ZSM-5 samples, in alkaline media, in where the named descriptors were varied one at the time, while maintaining the rest of the catalyst features constant. This methodology has allowed rationalizing the relative impact of each descriptor, as well as their interplay. The study showed that, firstly, square-shaped crystals with sub-micron sizes and Si/Al~300 limits the aromatic production, facilitate propylene diffusion and minimize the extension of consecutive reactions by shortening the length of both sinusoidal and straight channels and reducing the number of channel intersections, thereby maximizing propylene selectivity and life-time. Secondly, coffin-type crystals with crystal discontinuities showing diffusional restrictions [4], foster successive reactions leading to aromatics and faster decay. Finally, large coffin-shaped crystals with intergrowth particles also enhanced both propylene selectivity and catalyst life, in contrast to the commonly used large crystallites with bare surfaces, prepared under fluoride media, which deactivates faster. We hypothesize that this is due to a preferential orientation of the twinned subunits, which expose preferentially the sinusoidal pores and block the straight ones, [3] increasing the proportion of openings giving access to the zig-zag channels for the whole crystal. This allows more re-cracking events, but prevents the formation and/or diffusion of aromatic molecules and facilitate the diffusion of light hydrocarbons, such as propene, without being further converted into bulkier products or consumed in consecutive reactions in the straight pores. Thus, we showed that zeolite product shape-selectivity and catalyst life is affected by the preferential exposure of the intergrowth facets on the large crystallites.

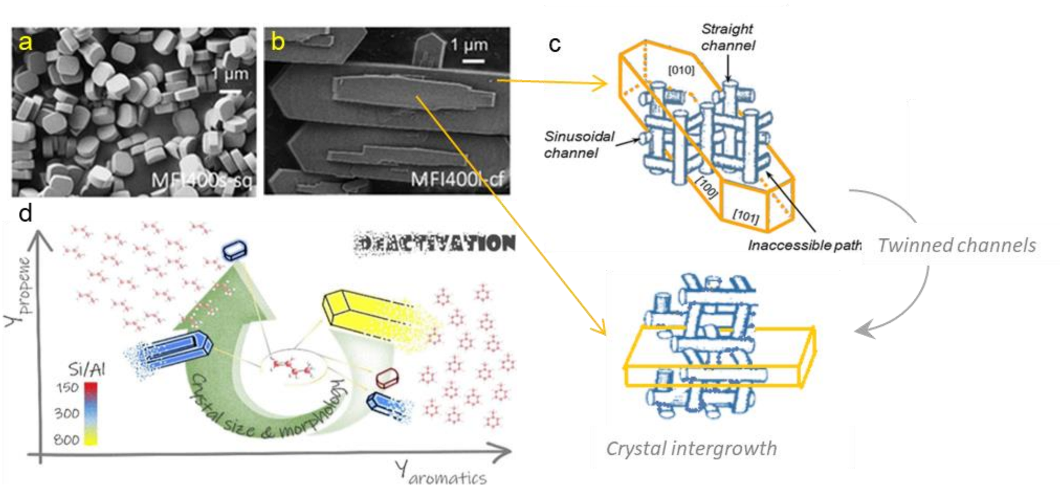

Fig.1. FESEM micrographs of small square (a) and large coffin-shaped with intergrowths (b) synthesized ZSM-5 crystallites and (c) projections of the channel orientations for a clean (top) and intergrowth (bottom) crystallite. Representation of the effect of diffusional (crystal size, morphology) and compositional (Si/Al) on the propylene yield and catalyst life.

Funding

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Acknowledgements

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P1 - Zeolite-Confinement of Alkaline Oxides for Selective Carbonate Catalysis

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Transesterification and related base-catalyzed alcohol addition reactions are central to sustainable chemistry, enabling the production of biodiesel and high-value organic carbonates such as ethyl methyl carbonate (EMC), a key intermediate for lithium-ion batteries and fuel applications. Here, we demonstrate that zeolite confinement combined with nanoscale oxide cluster design can overcome thermodynamic limitations in EMC synthesis from dimethyl carbonate (DMC). [1, 2]

While catalyst basicity governs DMC conversion, bulk inorganic oxides fail to achieve selectivity beyond equilibrium constraints. Here, we evaluated commercially available zeolites with distinct pore architectures and acid–base properties (H–USY, NaY, H-BETA, H-ZSM-5, and A-5) as catalytic nanoreactors. NaX zeolite exhibited superior performance, achieving 65% DMC conversion with 91% EMC selectivity, highlighting the influence of nanoscale confinement on reaction pathways. NaX also maintained stability over ten cycles and under continuous-flow operation. To further enhance activity, ultrasmall alkali and alkaline-earth oxide clusters (K_2O, Cs_2O, MgO, CaO) were introduced into NaX and NaY via wet impregnation and calcination. Characterization confirmed uniform dispersion of nanometric clusters within the pores without framework degradation. Catalytic evaluation revealed strong oxide-dependent effects: MgO@NaX increased conversion to 75% with 84% selectivity, while K_2O@NaX reached 93% conversion, surpassing thermodynamic equilibrium. These results demonstrate that the synergistic combination of zeolite confinement and nanoscale basic clusters offers a powerful strategy for selective and sustainable carbonate synthesis.

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P2 - Self-Supporting Films of Ordered Mesoporous Carbon based on Tailored Polyether Templates

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“Reverse Pluronic" block copolyethers ($PPO_{n/2}$-PEO_m-$PPO_{n/2}$) with tailored PPO block lengths (m = 90-450, $n/2$ = 20-200) were prepared using advanced, borane-based polymerization catalysis.[1-4] The resulting amphiphilic block copolyethers were then employed as nanostructure-directing agents in a soft-templating approach. The mesoporous structure is generated by organizing the block copolyethers in EtOH together with oligomerized phenolic resins (= carbon precursors) in an evaporation-induced self-assembly (EISA) process.[5-6] Subsequent thermal crosslinking (80-100 °C) and carbonization (600-700 °C) yields a series of mesoporous carbon materials (OMCs) with identical pore arrangement and comparable surface properties, differing only in their respective mesopore diameters (6-18 nm, depending on *m* and *n/2*). This well-defined, structural tunability renders the OMCs particularly suitable for the systematic investigation of confinement effects.[7]

In current work, these achievements are transferred to the preparation of self-supporting OMC films (~100 µm thickness, 1-10 cm^2 area). Essential parameters include pore arrangement (preferred: 3D-connected pore systems), pore size, mechanical stability of the films and the presence of surface functionalities for subsequent catalyst immobilization.[8] OMC films carrying covalently bound Fe- and Co-porphyrin catalysts are investigated as thin film electrodes or gas diffusion electrodes for the electrocatalytic reduction of CO_2, with the aim of selectively producing C^{2+} products.

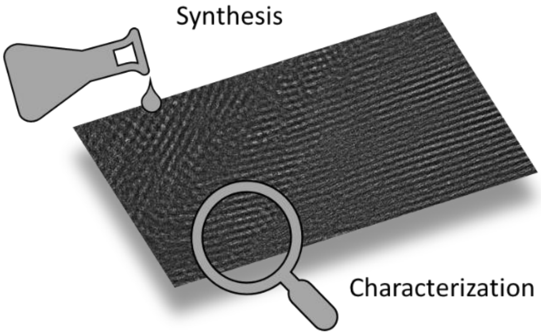

Fig.1. Schematic representation of a self-supported, ordered carbon film. [8]

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P3 - Synthesis of SBA-15 Mesoporous Silica from Sugarcane Bagasse Ash: Textural and Structural Characterization

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Mesoporous silica materials such as SBA-15 have attracted significant interest due to their high surface area, narrow pore size distribution, ordered hexagonal structure, and thermal stability, enabling a wide range of applications including adsorption, gas capture, catalyst, and use as support materials [1-3]. In recent years, increasing attention has been paid to the development of sustainable synthesis based on renewable silica sources. In this work, SBA-15 mesoporous silica was synthesized using silica extracted from sugarcane bagasse ash (SBA), an agro-industrial residue, as a sustainable precursor. Sugarcane bagasse ash was subjected to controlled heat treatment followed by acid leaching to remove inorganic impurities and increase silica content. Silica extraction from the treated sugarcane bagasse ash was carried out by a hydrothermal process using a 2 mol L^{-1} NaOH solution at a 1:15 (w/v) ratio and 120 °C for 6 h, achieving a SiO_2 extraction yield of 62.54 %. The extracted silica was used for the synthesis of SBA-15. The material obtained was characterized by nitrogen adsorption-desorption (BET), small angle X ray scattering (SAXS), infrared spectroscopy, scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The synthesized SBA-15 revealed a mesoporous nature with a high surface area (1095 m^2g^{-1}) and an average pore size of 4.1 nm, comparable to that of SBA-15 prepared from tetraethyl orthosilicate (TEOS). SAXS patterns and TEM images confirmed the presence of an ordered two-dimensional hexagonal mesostructure, while SEM images showed clustered, elongated particles. These results demonstrate the feasibility of valorizing sugarcane bagasse residues as an alternative silica source for the synthesis of ordered mesoporous materials comparable to those obtained from conventional precursors, with high potential in adsorption processes and as a functional support in advanced environmental and catalytic applications.

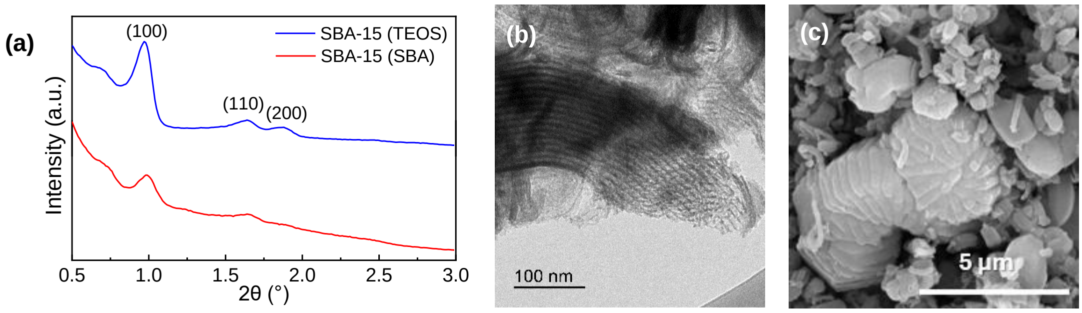

Fig.1. SAXS patterns (a), TEM images (b), and SEM images of SBA-15 (c).

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P4 - Unravelling the mechanism of photothermal catalytic CO_2 hydrogenation to methanol

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The photothermal catalytic hydrogenation of CO_2 to methanol represents a promising route for both carbon dioxide utilization and sustainable fuel production.[1, 2] This work aims to synthesize and characterize catalysts for methanol production. The focus is placed on CuZnAl (CZA) and CuZnZr (CZZ) catalysts, the former being an extensively studied benchmark system in the methanol synthesis literature, making the mechanistic insights broadly relevant to the catalysis community.[3, 4]

To optimize these well-established catalysts for photothermal applications, it is crucial to understand the underlying reaction mechanisms and identify active surface species under realistic operating conditions. To investigate this, an operando infrared spectroscopy investigation of CO_2 hydrogenation reactions over these heterogeneous catalysts was performed.

The experimental approach employs real-time FTIR measurements using a Harrick reaction cell capable of operation up to 400°C. This setup enables monitoring of surface-bound intermediates during CO_2 hydrogenation under controlled thermal conditions. The system is equipped with a tunable LED light source that provides wavelength-selective irradiation, allowing investigation of photocatalytic effects and deciphering the synergy between thermal and photochemical reaction pathways.

Initial operando IR measurements were performed at atmospheric pressure, targeting methane and carbon monoxide as the primary products.[5] The result was a clear identification of various reaction intermediates, particularly adsorbed methoxy species, which are expected to play a pivotal role in the methanol formation pathway.[6] These surface species provide valuable mechanistic insights even under conditions where methanol is not the final product. To validate the photocatalytic conversion of CO_2 to methanol, the catalysts were tested under conditions of elevated pressure (40 bar) and concentrated solar light, which are known to be favourable towards methanol synthesis.[6]

Initial operando infrared spectroscopy results will be presented, highlighting the identification and evolution of key surface intermediates, and discussing how these findings correlate with the first high-pressure validation experiments. This combined approach provides a comprehensive understanding of the photothermal CO_2 hydrogenation mechanism, bridging fundamental surface chemistry with practical methanol synthesis conditions.

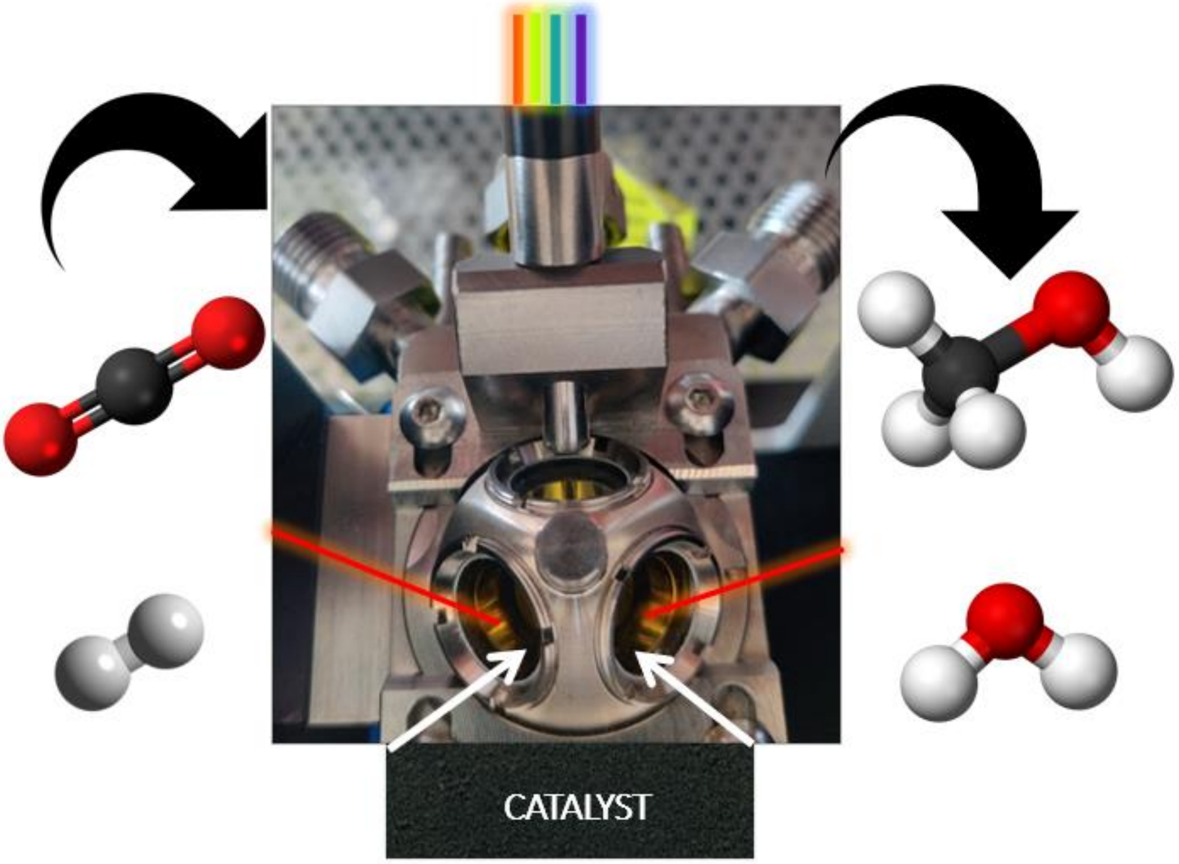

Fig.1. Graphical abstract.

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P5 - Beyond Solvents: Ionic Liquids as Architects of Copper Hybrid Functional Materials for Photocatalytic Hydrogen Generation.

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Ionic liquids (ILs) are typically viewed as auxiliary media, yet in advanced photocatalytic systems they can operate as true interfacial architects [1]. Here, we present a rapid and environmentally friendly strategy to construct copper hybrid functional materials for solar hydrogen generation, based on potassium hexaniobate hydrate ($K_4Nb_6O_{17}·xH_2O$, KNbO)[2] decorated with sputtered sub-nanometric copper clusters (SNCu)[3]. Despite an ultra-low copper loading of only 0.6 wt%, SNCu@KNbO already displays remarkable activity for hydrogen evolution under UV-Vis light. However, the decisive breakthrough arises when the material is encapsulated with the [BMIm][NTf_2], creating an engineered hybrid interface (IL@SNCu@KNbO) that simultaneously boosts activity, charge separation, and operational stability. The IL-architected photocatalyst reached 170 μmol of H_2 during alcohol photoreforming, equivalent to 4000 μmol g^{-1} h^{-1} (AQY=26.8%), clearly outperforming both SNCu@KNbO and KNbO. Spectroscopic and structural analyses reveal that the IL does not only coat the surface, but builds a polar nanolayer that reshapes the interfacial electronic structure, widens the band gap, broadens the valence band, and suppresses photoluminescence by nearly 80%, evidencing much more efficient charge-carrier management. At the same time, XPS and solid-state NMR confirm the chemical stability of the IL and its protective role against copper aggregation and photocorrosion. These findings position ILs as active design elements for copper-based hybrid photocatalysts, opening a new pathway for low-metal-loading, solvent-minimised, and highly efficient materials for sustainable hydrogen production.

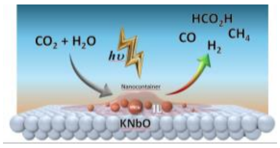

Fig.1. Schematic representation of the material presented in this work

Funding

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P6 - Electrocatalytic Copper radical reactions on nanostructured metal Oxides

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Radical reactions such as atom transfer radical cyclisation (ATRC) are powerful approach for building carbon-carbon bonds and cyclic molecules[1][2]. In typical systems, the copper catalyst is regenerated from Cu(II) to Cu(I) with sacrificial chemicals like ascorbic acid. These reductants often react with intermediates and products, causing side reactions, oligomers, and lower yields, especially at long reaction times.

In this work, we replace the chemical reductant with an electrochemical one. Copper complexes are immobilised on conductive ATO and ITO nanoparticles, which are nanostructured metal oxides with high surface area and good conductivity. By applying a potential, we precisely control the Cu(I)/Cu(II) redox cycle through this nanoporous oxide network. This gives access to more strongly reducing Cu species, improves the efficiency of ATRC and related radical additions, and clearly reduces parasitic reactions compared to the ascorbic acid system.

Overall, our results demonstrate that combining molecular copper catalysts with nanostructured ATO/ITO supports creates a tunable and sustainable platform for radical chemistry. The direct link between nanoporous conductive materials, controlled redox behaviour, and improved catalytic performance fits well with the ENMIX 2026 focus on nanoporous materials for advanced synthesis and functional applications.

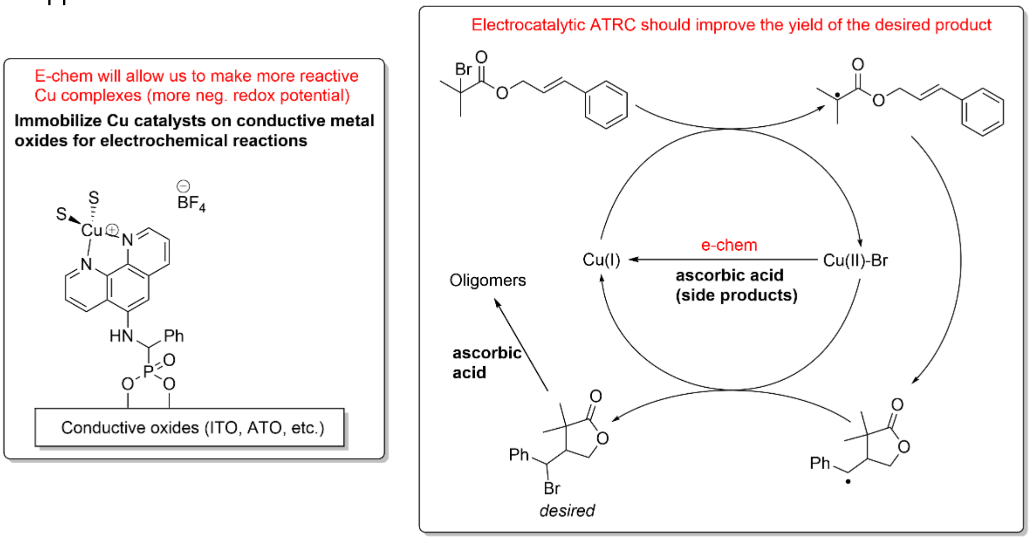

Fig. 1. Proposed ATRC reaction mechanism

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P7 - Engineering Rhenium–TiO_2 Interfaces for Low-Temperature CO_2 Methanol

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Developing efficient catalysts for green methanol synthesis via CO_2 hydrogenation is highly sought after. Although low temperatures and high pressures thermodynamically favor CO_2 conversion and methanol selectivity, catalyst design remains difficult due to limited CO_2 activation and low kinetic activity under such conditions. Re/TiO_2-based catalysts have demonstrated the ability to lower this kinetic barrier, achieving significant methanol production at temperatures as low as 150 °C and high pressures (50–330 bar)— substantially milder than the 200–250 °C typically required by industrial Cu/ZnO/(Al_2O_3) catalysts.[1,2] The exceptional performance of these Re-based systems is attributed to two key features: (i) a size-dependent catalytic behavior, where sub-nanometer Re clusters promote methanol formation, while isolated Re atoms and larger Re particles tend to favor CO and CH_4 production, respectively (Figure 1a); and (ii) a unique redox flexibility that enables the coexistence of highly dispersed cationic Re species and metallic Re clusters. This dual nature facilitates the simultaneous formation of reactive Re–hydride and Re–carbonyl species, which are responsible for generating and activating key intermediates (e.g., formates) that ultimately lead to high methanol selectivity.[1,2]

A systematic evaluation of Re/TiO_2 catalysts with Re loadings between 3 and 50 wt% was conducted under CO_2 hydrogenation conditions (300 bar, 35–200 °C). Remarkably, methanol formation was detected at temperatures as low as 35–50 °C, reaching >60% selectivity—performance not previously reported for CO_2 hydrogenation catalysts. Increasing Re loading above ~24 wt% enhanced methanol selectivity at low temperatures (<100 °C), whereas higher temperatures promoted CH formation at the expense of methanol. TEM (Figure 1b) and XRD (not shown) analyses of the 48 wt% Re/TiO_2 sample revealed no large Re aggregates even at elevated loadings. Operando DRIFTS during CO hydrogenation showed distinct linear Re–CO bands (2075 and 2035 cm^{-1}) (Figure 1c), confirming the presence of low nuclearity Re species analogous to those observed in low-loaded systems. These results, together with in-situ XAS studies, suggest that the enhanced low-temperature activity originates from highly dispersed Re sites capable of stabilizing reactive carbonyls.

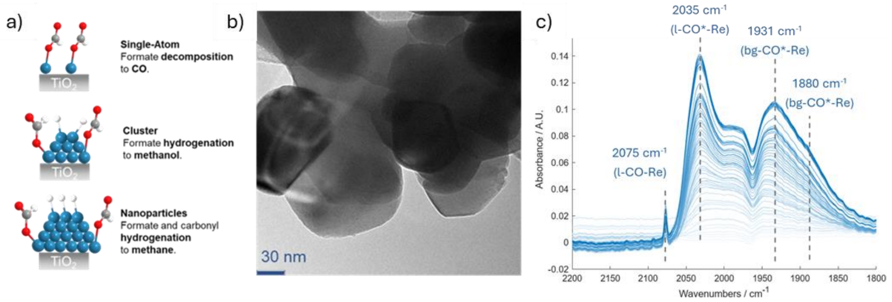

Figure 1. a) Schematic illustration of the proposed size-dependent catalytic behavior of Re/TiO_2 catalysts. b) TEM micrograph of a 48 wt% Re/TiO_2 catalyst after calcination in air at 350 °C under atmospheric pressure, showing no visible Re aggregation. c) Time evolution *operando* DRIFT spectra of the carbonyl region under CO_2 hydrogenation conditions (10 bar, H_2:CO_2=3, T=50°C).

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P8 - Co@C Nanoparticles as efficient catalysts for magnetic induction heating-assisted hydrogenation of lactic acid

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Biomass upgrading has attracted significant research interest because it enables the conversion of renewable feedstocks into valuable chemicals and fuels. The hydrogenation of lactic acid (LA) is commonly carried out using Ru-based catalysts, which underscores the importance of developing efficient catalysts based on non-noble metals to lower costs and enhance the overall sustainability of the process [1]. Magnetic induction heating (MIH) has been shown to achieve higher conversion rates compared with conventional heating techniques, while also enabling improved control over hydrogenation selectivity. This approach is based on the application of an alternating magnetic field that interacts with magnetic nanoparticles, generating localized heat. Consequently, the catalyst functions simultaneously as both the heat source and the active catalytic phase [2]. In this study, cobalt magnetic nanoparticles coated with a carbon layer were synthesized through the catalytic graphitization of cellulose. The catalyst synthesis was performed through the wet impregnation of cellulose with $Co(NO_3)_2.6H_2O$, and urea (for Co@N-C), and without urea for Co@C. The mixtures were dried using a rotary evaporator, followed by oven drying at 100 ºC and pyrolysis at 700 ºC for 3h under a 20 mL/min N_2 flow. TEM analysis revealed the formation of homogeneously distributed magnetic Co nanoparticles with an average particle size of 9.0 ± 1.06 nm on the surface of a carbonaceous support. XRD patterns displayed the characteristic graphite (002) reflection together with the Co *fcc* (111) peak, with no detectable signals corresponding to oxidized Co species, in agreement with the Raman spectroscopy results.

The catalysts were evaluated in the hydrogenation of LA under magnetic induction heating (MIH) in aqueous media, using 50 mg of catalyst (10 wt% Co) under 10 bar of H_2, a magnetic field amplitude of 63 mT, and a local temperature (T_{local}) of 160 °C. The catalytic results showed that Co@NC was inactive, likely due to strong carbon–nitrogen interactions that limit the accessibility of active sites. In contrast, Co@C achieved 96% LA conversion after 6 h. The product distribution consisted mainly of propanoic acid (PA, 88%), along with minor amounts of 1,2-propanediol (1,2-PD, 4%), 1-propanol (1-P, 2%), and isopropanol (IPA, 6%). After 18 h, PA selectivity decreased to 69%, accompanied by the formation of 1,2-PD (2%), 1-propanol (1-P, 20%), and isopropanol (IPA, 9%). These results demonstrate that product selectivity under MIH can be effectively tuned by adjusting the reaction time. Reusability tests showed that Co@C remained catalytically active after six consecutive cycles. Raman spectroscopy of the spent catalyst revealed the presence of oxidized Co species, while TEM analysis indicated a slight increase in particle size from 9 to 13 nm, likely due to particle sintering. In contrast, under conventional heating at 190 °C, the reaction reached only 63% LA conversion after 6 h, with propanoic acid (PA) as the sole product. Furthermore, the surface temperature (T_{surf}), corresponding to the actual temperature at the Co nanoparticle surface, was estimated using the Arrhenius equation and found to be 220 °C, significantly higher than the measured T_{local} of 160 °C. This result highlights the ability of MIH to generate higher localized temperatures, thereby enhancing the catalytic conversion of the material.

Acknowledgements

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P9 - Synthesis of Co Nanoparticles Confined in N-doped Carbon for CO_2 Valorization via the Reverse Water-Gas Shift Reaction.

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Catalytic valorization of CO_2 into value-added products represents a promising strategy to mitigate greenhouse gas emissions and advance sustainable chemical processes [1]. Among the available routes, the Reverse Water–Gas Shift (RWGS) reaction enables the selective production of CO, a key intermediate for downstream technologies such as Fischer–Tropsch synthesis [2]. However, developing active and stable catalysts remains challenging due to the competition with methanation and metal sintering under reaction conditions [3].

Herein, we report the synthesis of cobalt nanoparticles encapsulated within N-doped carbon matrices, where the pyrolysis temperature was systematically tuned to control the carbon structure, metal dispersion, and stabilization of the active species. The catalytic performance of ***Co@MelCit-X*** (X = 700, 750, and 800 °C) was evaluated between 450–600 °C, maintaining a constant temperature for 1 h for each analysis, and increasing it by 50 °C per segment. The reaction was conducted in a continuous-flow stainless-steel reactor using a 4:1 H_2:CO_2 molar ratio, a total flow rate of 100 mL/min, and a GHSV of 120 L $gcat^{-1}$ h^{-1}. The gases were analyzed online using a Pfeiffer OmniStar GSD 301 GC-MS system.

Characterization results indicate that the pyrolysis temperature plays a decisive role in defining the catalyst architecture. N_2 adsorption–desorption analysis revealed a pronounced textural evolution: while the sample treated at 700 °C exhibited a nearly non-porous morphology (S_{BET} = 14 m^2 g^{-1}), increasing the temperature to 800 °C led to the formation of a highly developed mesoporous structure with a surface area of 512 m^2 g^{-1}. XRD patterns display a broad diffraction peak at ~26°, assigned to the (002) plane of graphitic carbon, confirming partial graphitization at high temperature. A weak contribution around 44° suggests the presence of metallic cobalt domains (Co^0), although peak overlap with carbon reflections and the low crystallinity of confined nanoparticles hinder definitive phase identification. The combined TEM and XPS analyses support the presence of metallic cobalt nanoparticles partially encapsulated within a graphitic N-doped carbon matrix. Although surface oxidation generates Co^{2+} species, the nanoparticle core remains in a reduced state, stabilized by the nitrogen-doped carbon framework.

Regarding catalytic performance, the ***Co@MelCit-800*** catalyst exhibited superior activity, reaching a CO_2 conversion of approximately 15% at 600 °C. Remarkably, this catalyst maintained near 100% CO selectivity throughout the entire temperature range, completely suppressing the methanation pathway. These results suggest that the synergistic effect between high surface area, turbostratic carbon structure, and nitrogen-mediated metal stabilization is key to achieving efficient and selective RWGS performance.

Funding

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P10 - Macrostructured carbon based architectures as key-solution for advanced water treatment

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Heterogeneous catalysis applied to water treatment has been widely studied for the removal/conversion of several organic and inorganic contaminants present in water using adequate catalysts to promote the reaction. Although most of the studies have been conducted at laboratory scale, increasing attention is being given to their transition to industrial application [1]. This transition has been accompanied by the development of immobilization techniques that ensure proper incorporation of active catalysts into treatment systems, avoiding the pressure drop issue commonly associated with the use of powder catalysts in continuous reactors [2].

The present work focuses on the development and application of macrostructured carbon-based catalysts in an integrated system designed for the simultaneous removal of organic and inorganic contaminants from water. The catalysts were prepared using two main approaches: washcoating using two distinct surfactants (Triton X-100 as a conventional surfactant and sodium alginate (SA) as a greener alternative) and chemical vapor deposition (CVD) as a traditional method for the preparation of carbon macrostructured catalysts. In this context, carbon-based catalysts were applied in the ozonation stage (WCP_550 and WCP$_{SA}$_550), while bimetallic catalysts supported on carbon materials were used in the reduction step (WCP(CNT:TiO$_2$)_550_Pd_200_Cu, WCP(CNT:TiO$_2$)$_{SA}$_550_Pd_200_Cu and CVD_Pd_200_Cu) [3,4].

Both preparation methods produced stable macrostructured catalysts. Washcoating enabled the immobilization of about 2 % carbon material and allowed the effective incorporation of modified CNT powders (CNT(BM 2h) and CNT:TiO$_2$), preserving their surface chemistry and modifications. In contrast, CVD led to carbon nanofiber growth of about 4 %.

All catalysts showed high activity and stability for around 30 h during the treatment of surface water, showing complete degradation of the detected organic micropollutants (during catalytic ozonation), while mitigating and converting BrO_3^- formed during the previous treatment to levels below the advised legal limit for its presence in water, showing, this way, comparable results independently of the synthesis methodology. A life cycle assessment of the macrostructured catalyst synthesis showed that the washcoating method reduced environmental impacts by 30–50% compared with conventional methods, while maintaining catalytic performance.

Acknowledgements

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P11 - Influence Of Ge On The Crystallization Of Zeolite ITQ-13 Studied By Solid State NMR

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Introduction

Zeolite ITQ-13 exhibits an ITH-type framework composed of three intersecting medium-pore channels (9 × 10 × 10 Å) and may form intergrowths with the ITR structure [1]. The ITH framework contains *d4r, stf, lau*, and *mel* cages. When synthesized in the presence of HF, fluoride anions compensate the OSDA cations and are mainly located in the *d4r* and *mel* cages [2]. The incorporation of germanium into the synthesis gel leads to partial Si substitution in the framework, preferentially at sites forming *d4r* units.
This work aims to elucidate the roles of fluoride and germanium during ITQ-13 crystallisation, focusing on the time-resolved distribution of fluoride among ITH cages as studied by solid-state NMR and XRD.

Results and discussion

Gels with Si/Ge ratios of 3, 6, and 25 were synthesized and treated hydrothermally at 175 °C for 1–15 days.
For Si/Ge ≈ 3, the BEC polymorph forms at early crystallization stages (1–2 days), while the ITH phase appears at longer times, although BEC remains dominant. Fluoride content increases with time, and ^{19}F NMR spectra show fluoride in *d4r* units (the only one present in the BEC) throughout, with signals from *mel* cages appearing only at later stages. For Si/Ge ≈ 6, BEC and ITH coexist initially, but pure ITH is obtained at long crystallization time. Fluoride is detected in both *d4r* and *mel* cages, and its content evolves non-linearly over time, indicating phase transformations. For Si/Ge ≈ 25, EUO and ITH form at early times, whereas pure ITQ-13 is achieved at 15 days of crystallization, accompanied by an increase in fluoride content and stronger ^{19}F NMR signals from fluoride in pure-silica and mono-germanium *d4r* cages.
The zeolite phases obtained from Si–Ge synthesis gels depend strongly on germanium content and crystallisation time. For Si/Ge=3, the C polymorph of beta zeolite (BEC) containing uniquely *d4r* cages, is consistently formed reflecting the ability of Ge to stabilise *d4r*-rich frameworks at early stages. At higher Si/Ge ratios (6 and 25), pure ITQ-13 is obtained only at long crystallisation times, whereas shorter times yield mixtures with BEC or EUO. The non-monotonic evolution of fluoride content is attributed to phase transformations during crystallisation.

Acknowledgments

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P12 - Exploiting confinement effects for urea electrosynthesis from CO_2 and nitrate using covalent organic frameworks (COF) as substrate.

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Electrochemical CO_2/nitrate co-reduction offers a low-carbon alternative under ambient conditions. This approach valorises industrial CO_2 and nitrogen pollutants, thereby advancing a sustainable circular carbon-nitrogen economy. In this project, COF-based catalyst architectures are developed to exploit molecular confinement effects for controlling the co-reduction of CO_2 and nitrate. For urea formation, C=O and N=O bond cleavage occurs alongside selective C–N coupling of surface-bound intermediates. Additionally, kinetically challenging side reactions compete, including direct eCO_2RR pathways and parasitic HER. Hence, making it necessary for the dedicated catalytic sites for CO_2 and NO_3^- activation to be precisely Ångström-scale in proximity to favour the coupling of $^*CO$ and $^*NH_2$ intermediates eventually. The spatial arrangement of catalytic centres, as defined, is designed to increase the coupling probability. Such a catalytic system would optimise proton–electron coupling and suppress parasitic reactions. For catalytic performance, the catalyst will be evaluated in both H-type cells and flow-cell configurations employing COF-modified gas diffusion electrodes (GDE), allowing us to correlate confinement-induced changes in activity, selectivity, and urea yield. Our continuum modelling would be adapted for this project to rationalise macroscopic performance against the local microenvironment[1]. Operando electrochemical impedance spectroscopy (EIS) would be used to deconvolute different processes in-situ[2]. This multi-scale approach elucidates structure–activity relationships. It establishes design rules for nanoconfined, multi-component COF electrocatalysts targeting >90% Faradaic efficiency to urea, as benchmarked in recent Fe-porphyrin COF reports[3].

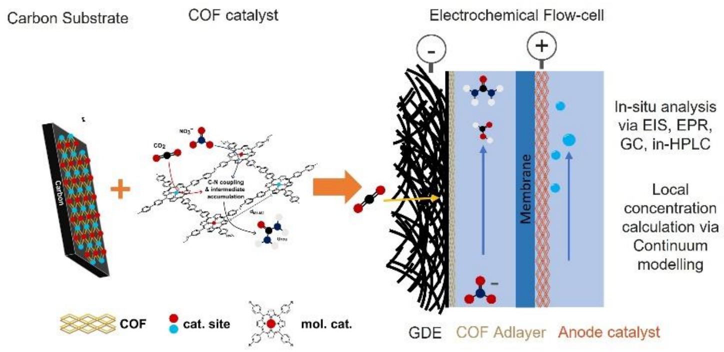

Fig. 2. Integrated COF-GDE approach for Urea electrosynthesis.

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P13 - Integrated CO_2 Capture and Methanation under Realistic Conditions: Na as Key Promoter in Ru/Mg–Al DFMs

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Integrated CO_2 capture and methanation (ICCM) using dual-function materials (DFMs) represents a promising strategy for flexible power-to-gas applications and CO_2 valorisation [1]. For practical implementation, DFMs must simultaneously ensure high CO_2 storage capacity and rapid, selective methane formation under cyclic operation, particularly when realistic feeds containing H_2O and O_2 are employed [2]. In this study, a Ru-based DFM supported on a hydrotalcite-derived Mg-Al oxide and promoted with Na (Ru/Na-Mg-Al) is investigated for isothermal ICCM in a fixed-bed reactor. This novel formulation, not previously explored for this operating mode, is compared with unpromoted (Ru/Mg-Al) and K-promoted analogues (Ru/K-Mg-Al) to elucidate the role of alkali metals on CO_2 adsorption, hydrogenation kinetics and cyclic performances under both ideal conditions (5% CO_2/N_2) and simulated realistic flue-gas compositions including H_2O and O_2 during the capture stage. A combined experimental approach integrating cyclic CO_2 capture and H_2-TPSR in TG-MS, fixed-bed cyclic methanation tests, and in situ DRIFTS was employed to link surface intermediates with macroscopic performance. Na promotion significantly enhances CO_2 capture and enables fast and selective CH_4 production, outperforming benchmark materials (Ru/Mg-Al and Ru/K-Mg-Al). While Ru/Mg-Al shows higher intrinsic methanation rates but insufficient adsorption capacity, and K promotion favours stable surface species and increased CO formation, Na generates a reactive pool of carbonates, formates, and carbonyls persisting after isothermal purge and progressively converted into methane. Methanation is initially rapid but becomes limited at longer times by slow surface diffusion of stored species toward Ru active sites. Parametric tests demonstrate that O_2 in the capture step reduces cyclic CH_4 yield by 10-15% (Figure 1) by delaying the restoration of metallic Ru at the start of hydrogenation, where most methane is produced. Water exhibits a dual role, increasing CO_2 storage through activation of MgO adsorption sites while moderating initial methanation kinetics and improving CH_4 selectivity, leading to a net effect strongly dependent on temperature and cycle duration.

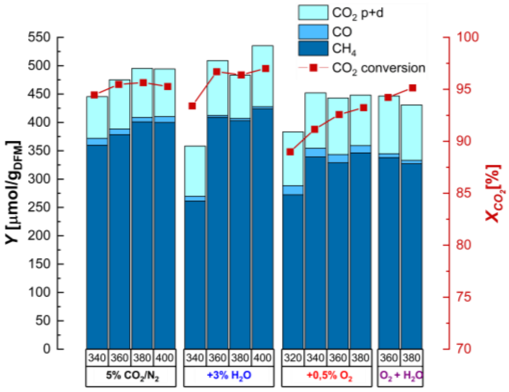

Figure 1. Effect of the feed gas composition and reaction temperature during the ICCM with Ru/Na-Mg-A DFM on average values of CH_4 and CO produced, the sum of CO_2 purged and desorbed, and CO_2 conversion obtained during 3 consecutive cycles.

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P14 - Breaking the Activity–Stability Trade-Off in CO Oxidation Catalysis: Insights from Pt on Reducible and Non-Reducible Supports

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Supported Pt catalysts are widely used for CO oxidation, but their performance strongly depends on the support. Redox-active supports such as CeO_2 promote highly active metal–support interfaces via lattice oxygen participation, yet they often deactivate under O_2-rich conditions due to oxidative fragmentation of Pt nanoparticles into less active isolated Pt atoms.

Conversely, non-reducible supports such as siliceous zeolites enhance the structural stability of subnanometric metal clusters by suppressing oxidative redispersion and sintering. In K-doped MFI zeolites, small Pt clusters (~1 nm) can be stabilized at defective framework sites and electronically promoted by alkali cations, generating electron-rich Pt ensembles capable of activating CO and O_2. However, the absence of redox functionality typically limits their catalytic activity compared with Pt/CeO_2 systems.[1]

Here, we analyze how the nature of the support controls the structure and reactivity of Pt species in CO oxidation by comparing Pt catalysts on reducible (CeO_2) and non-reducible (zeolite) supports. By engineering the metal–support interface in ceria, we stabilize small metallic Pt nanoparticles at specific surface sites that suppress oxidative redispersion while preserving metal–ceria cooperation. This strategy breaks the conventional activity–stability trade-off in Pt catalysts, enabling high turnover frequencies together with remarkable stability under O_2-rich conditions.[2]

These results highlight the decisive role of support redox chemistry, metal nuclearity, and metal–support interactions in determining catalytic performance.

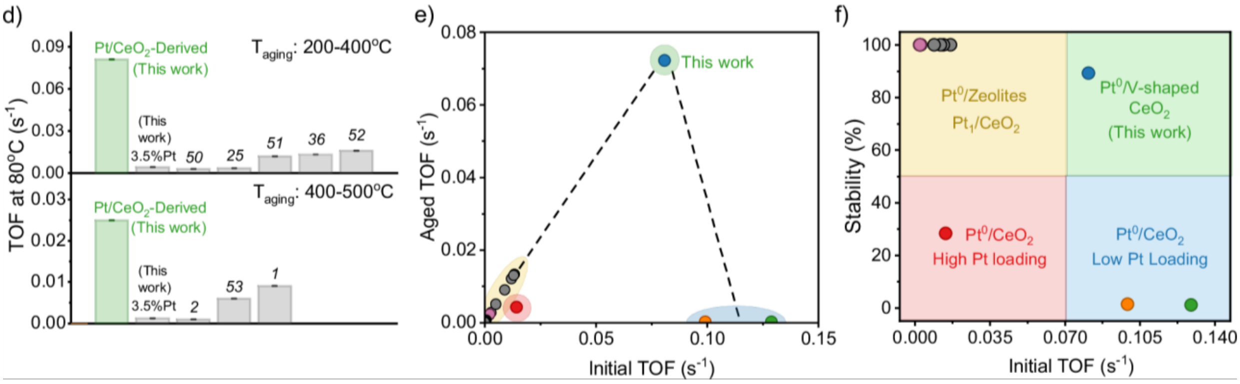

Fig.1. (d–f) Comparison of CO oxidation performance for representative Pt catalysts after aging in O_2-rich streams. The plots relate initial activity, aged activity, and stability, illustrating the common activity–stability trade-off and showing that the Pt/CeO_2-Derived catalyst (this work) uniquely combines both high activity and high stability.

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P15 - Engineering BiOBr/g-C_3N_4 Heterostructures for Visible-Light Photocatalytic Valorization of Biomass-Derived Compounds

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Biomass energy plays a pivotal role in the transition to low carbon within the energy sector and can be used to produce the fundamental organic chemical feedstock. Among biomass-derived compounds, 5-Hydroxymethylfurfural (HMF) is a key oxygenated compound that can be selectively converted into high-value compounds. Its oxidation can yield diformylfuran (DFF), a valuable intermediate widely used as a precursor in the synthesis of fine chemicals, pharmaceuticals, and polymer materials.

Photocatalysis has emerged as a promising sustainable technology for biomass valorisation, enabling the use of solar energy, mild reaction conditions (ambient temperature and pressure), and the possibility of operating in aqueous media. However, developing cost-effective, chemically stable, and highly active photocatalysts capable of operating under visible light remains a challenge for practical application.

Among visible-light-responsive semiconductor photocatalysts, bismuth oxyhalides (BiOX, X = Cl, Br, I) and graphitic carbon nitride (g-C_3N_4) have attracted considerable attention. BiOBr is particularly interesting due to its unique layered structure, high chemical stability, and a suitable bandgap for visible-light activity [1]. Meanwhile, g-C_3N_4 is a low-cost and metal-free semiconductor with high thermal and chemical stability and a non-toxic nature [2]. Despite these advantages, its practical performance remains limited by its low surface area and the rapid recombination of photogenerated electron-hole pairs.

In this work, BiOBr/g-C_3N_4 composites were synthesised to enhance their photocatalytic performance under visible-light irradiation. The influence of BiOBr content on the optical properties of g-C_3N_4 was investigated. The results show that increasing the BiOBr content in the g-C_3N_4 structure led to a blueshift in absorption and a decrease in photoluminescence intensity, indicating improved charge separation. Photocatalytic tests demonstrated that the composite material containing 30 wt% BiOBr increased HMF conversion and DFF yield by two times in aqueous medium, operating in batch mode, compared to pristine g-C_3N_4. Radical quenching experiments were performed to identify the main reactive species involved in the photocatalytic oxidation mechanism.

Acknowledgements

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P16 - Design Of Bi-Functional Ni-Zeolites For Ethylene Oligomerization: Controlling Zeolite Properties By One-Pot And Post-Synthetic Ni Incorporation

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Light olefins ($C_2^=$-$C_6^=$) are considered to be important intermediates for the synthesis of various organic product, fuels, and solvents. More specifically, the oligomerization of light olefins has drawn an industrial interest due to the flexibility of selecting the starting material as well as the range of the molecular weight of the final product [1]. Acid zeolites have been extensively employed as efficient heterogeneous oligomerization catalysts when using propylene or higher olefins but, in the case of ethylene, the incorporation of transition metals enables the activation and conversion of the olefin under moderate temperature conditions [2]. Nickel is the most studied metal and traditionally post-synthesis ion-exchange, or impregnation methods are used for its addition to the zeolite-based support.

Here we present the rational design of a set of Ni-containing zeolites based on two crystalline structures, BEA and MFI, where the chemical composition (Si/Al ratios from 10 to 40) and Ni incorporation (by conventional post-synthesis impregnation and by one-pot synthesis employing N-ligands) were studied [3]. The samples have been thoroughly characterized and their catalytic behavior has been compared with that of commercial MFI and BEA with comparable Ni loadings in the oligomerization of ethylene to heavier olefins. Catalytic tests have been performed in a fixed-bed reactor under two different condition sets: 2.5 bar, 180ºC, 16.3 h^{-1} and 2.5 vol% C_2H_4 and 35 bar, 200ºC, 2.1 h^{-1} and 15 vol% C_2H_4.

According to the characterization results obtained for the different Ni-zeolites prepared, the formation of NiO nanoclusters inside the zeolitic pores is favored by the one-pot synthesis of nanocrystalline Ni-zeolites, while nickel incorporation by post-synthesis impregnation lead to higher contents of cationic Ni^{2+} in ion exchange positions, species that are better stabilized for zeolites with higher Al contents.

Regarding the catalytic behavior of these samples, when working under near ambient pressure, low partial pressure and high space velocity, crystal size does not play a decisive role, and catalysts prepared by post-synthesis methods are more active due to the higher amount of Ni^{2+} species. When reaction is performed under higher pressures and higher ethylene/catalyst ratios, more representative of industrial operation, other factors besides Ni speciation play an important role in the catalytic behavior of the bifuncional Ni-catalysts. Thus, the nano-sized zeolites are more active and more stable towards deactivation than the commercial-based catalysts with larger crystals (see Figure 1) and present a higher selectivity to C_{5+} hydrocarbons and one-pot Ni incorporation increases even more the yields to heavier oligomers.

Acknowledgements

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P17 - Electrochemical CO_2 Reduction under Nanoconfinement: CO_2-reduction with molecular catalysts immobilized on ordered mesoporous carbons

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The electrochemical reduction of CO_2 (CO_2RR) is strongly influenced by the structural and chemical properties of the electrode material, including pore architecture, surface functionality, and electrolyte accessibility. Ordered mesoporous carbons (OMCs) provide a versatile platform to study nanoconfinement effects, as their pore size, surface chemistry, and catalyst distribution can be systematically tailored.

In this work, organometallic molecular catalysts are combined with OMCs to investigate how confinement within mesoporous carbon networks affects electrocatalytic performance[1]. The molecular catalysts are first evaluated in solution, where well-defined electrochemical behavior and CO formation are observed. To integrate these catalysts into porous carbon architectures, different immobilization strategies are explored, including pore-selective tethering and incipient wetness impregnation (IWI). While selective tethering aims to localize active sites exclusively inside the mesopores, its experimental realization and verification remain challenging. The resulting materials are evaluated using both conventional H-type cells and gas diffusion electrode (GDE) configurations, enabling systematic comparison between planar and nanoconfined porous electrodes. This materials-focused approach provides insight into how pore structure, surface chemistry, and catalyst distribution govern activity and selectivity, contributing to a mechanistic understanding of CO_2RR in nanoconfined porous carbon electrodes.

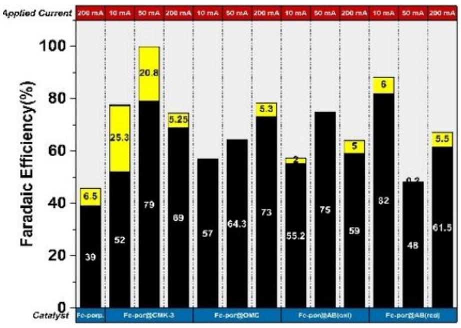

Fig.1. Faradaic efficiencies of tethered organometallic catalysts under aqueous conditions.

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P18 - O,P Codoping as a Strategy to Balance Photocatalytic Performance Toward Multi-Pollutant Applications

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The application of photocatalysis to wastewater treatment demands catalytic systems that maintain activity across structurally diverse pollutants [1]. Building on this premise, this work explores O,P-codoping of SWCNT-modified TiO_2 as a compositional approach to extend photocatalytic applicability to heterogenous wastewater matrices under simulated sunlight irradiation. Synthesis optimization strategies targeted parameters like heteroatom ratio and pyrolysis temperature, while catalytic performance was evaluated using rhodamine B, ibuprofen, and imidacloprid as representatives of chemical and functionally distinct pollutant categories. Overall, spectroscopic analysis (XPS, Raman) confirmed successful heteroatom incorporation, and preservation of the SWCNT framework throughout functionalization process. Whereas XRD and BET measurements verified TiO_2 crystallinity and showed comparable surface areas across all composites. Interestingly, increasing phosphorus content (2:1, 4:1, and 6:1 wt.%) led to progressively higher hydrophilicity, as evidenced by immersion calorimetry (54.7, 67.1, and 80.6 $J{\cdot}g^{-1}$). This trend correlates with the selective increase in CO evolution observed by TGA–MS (Ar), indicating enhanced formation of defect-related oxygen functionalities and P–O–C environments [2]. On the other hand, changes in pyrolysis temperature significantly influenced the specific phosphorus group developed and its retention on the carbon matrix. Correlative XPS and ICP-MS analyses showed that higher treatment temperatures reduced phosphorus lixiviation during the oxidation step, indicating improved stabilization on the nanotube surface. This behavior was consistent with TGA (Ar) results, which confirmed enhanced thermal stability at elevated pyrolysis temperatures, slightly reinforced after codoping process. These parametric variations translated into a robust photocatalyst able to degrade 90% of all tested pollutants within five hours of irradiation. Overall, the highest phosphorus content (OPC_6:1) formed as $C–PO_3$ functionalities at 800 °C, delivered the most favorable photocatalytic performance. When tested throughout 5 consecutive cycles for each pollutant, the catalyst maintained a stable response with minimal activity loss. It's also worth noting that direct benchmarking against monodoped references confirmed that activity differences are more sensitive to heteroatom-derived surface chemistry rather than synthesis parameters. Therefore, codoping preferentially promotes balanced photoactivity across distinct degradation pathways.

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P19 - Hydrophobic Zeolites for Direct Air Capture

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The EU project eREGENERATE (**RE**sistive heatin**G** in structured hydrophobic sorbents for a highly **E**fficie**N**t and fully **E**lectrified Di**R**ect **A**ir Cap**T**ur**E** technology) has the goal to develop a novel Direct Air Capture (DAC) technology based on cost effective and long-lasting sorbents, as well as a novel fully electrified process technology. The project will elaborate on a roadmap to ensure scale up and deployment of eREGENERATE technology in the European and Canadian markets. The industrial DAC partner in the consortium, Removr, plans to deploy the innovations in their large-scale DAC plants. More specifically, the project aims at addressing current DAC challenges using four key innovations. The first innovation involves synthesizing and scaling up hydrophobic zeolites, a sorbent with a long lifetime, capable of capturing CO_2 at low concentrations and in the presence of water (i.e., humid air), to ensure high capturing performance coupled with low manufacturing cost. The second innovation introduces an electrically conductive substrate on which the zeolite will be coated, giving low pressure drop (hence low energy consumption in adsorption) and fast heating of the adsorbent bed to desorb the CO_2. The third innovation is a new electrical swing process, fully powered by renewable energy. The fourth innovation is a first-of-a-kind algorithm able to optimise the complete chain of capture and conditioning of the CO_2, as well as assessment of the energy source mix and weather impact on it, to overcome the strong energy intensity of the capture process and optimise both energy input and purity in between the capture process and the conditioning step. Further, to ensure the technology's success and societal acceptance, a structured stakeholder engagement process will be elaborated all along the technological development to co-create strategies, including policy and incentives, to align DAC deployment with societal priorities.

The University of Stuttgart will develop together with SINTEF the hydrophobic sorbents, which should have a higher water tolerance with stable DAC performance so that the thermal regeneration of the zeolite can be avoided in a pre-bed configuration for dehumidification. Core/shell structures with a hydrophilic core and a hydrophobic shell will be made, e.g., with mild dealumination procedures. In addition, the University of Stuttgart will in a joint activity with Johnson Matthey coat these sorbents onto electrically heatable coupons for testing. These results are later transferable to monoliths for the pilot-scale testing.

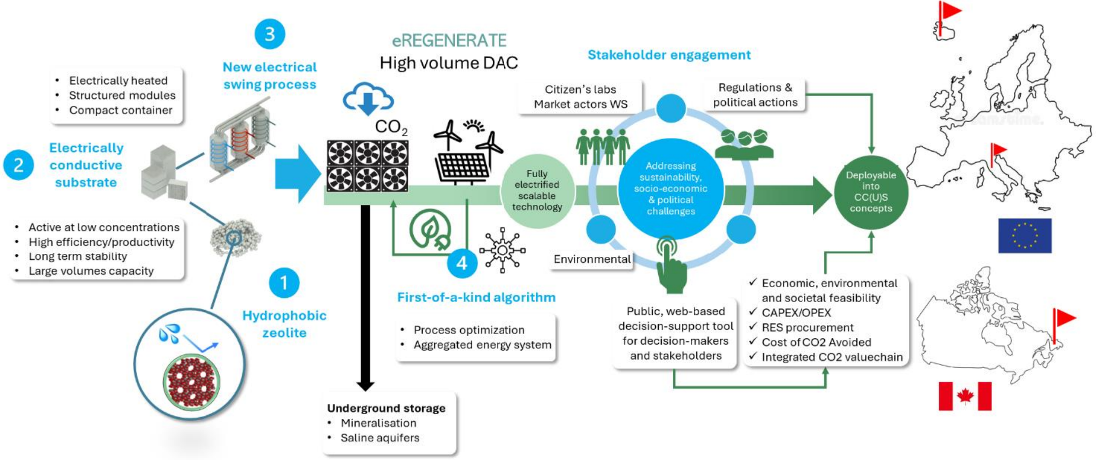

Fig.1. eREGENERATE project concept.

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P20 - Hybrid Pd-In/MOx photocatalysts for hydrogen production by alcohol photo reforming using simulated sunlight

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In this work, nano-structured hybrid systems based on bimetallic Pd-In particles supported on photoactive semiconductor oxides (TiO_2, Nb_2O_5 and WO_3) were designed and developed with potential application in the production of green hydrogen under simulated solar irradiation. The study includes the synthesis of nanomaterials, evaluation of their photocatalytic activity, and structural, chemical and photophysical characterization of the most active systems. Additionally, the photosensitizing effect of ionic liquid 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ($BMIm.NTf_2$) over the most active system was evaluated [2] [3].

The synthetic strategy was based on the solvothermal growth of metal-organic frameworks (MOFs) over three different semiconductors (PdInMOF@SC) [1], followed by a chemical-thermal treatment to generate highly dispersed Pd-In nanoparticles (PdInQT@SC) with an average size of between 5-10 nm.

The characterization of materials was carried out using advanced techniques with the aim of correlating their composition, structure, and photoelectronic properties with photocatalytic performance. The activity was evaluated in a quartz reactor under irradiation with a UV-Visible light lamp, while the gaseous products were analyzed by gas chromatography.

The PdInQT@TiO_2 system presented the highest efficiency for hydrogen evolution, reaching up to 140 µMol.g^{-1} of H_2 per gram of catalyst in the methanol photo reforming and up to 150 µMol.g^{-1} of H_2 per gram of catalyst in glycerol photoreforming after 4 h of total irradiation. In contrast, the systems based on Nb_2O_5 and WO_3 showed no appreciable production of H_2 under the evaluated conditions. The results show that the encapsulation of the most active system with the IL promoted the reaction in methanol, increasing the evolution of H_2, while in the glycerol a decrease in activity was observed attributed to diffusional limitations on the surface.

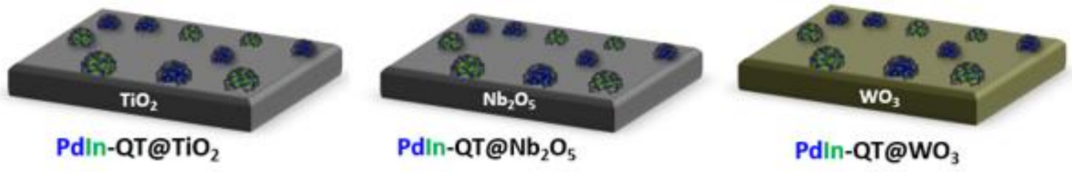

Fig.1. Graphic representation of synthesized materials evaluated in this work

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P21 - Coke-Induced Deactivation of HZSM-5 during Continuous Pyrolysis and Catalytic Cracking of Biomass-Derived Volatiles

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Bio-oils obtained from the thermal pyrolysis of lignocellulosic biomass are unsuitable for any direct application due to their unfavorable physicochemical properties, including high acidity and oxygen content, chemical instability, presence of impurities, and strong tendency toward polymerization [1]. An upgrading step is therefore mandatory to improve fuel quality. Among the available upgrading strategies, catalytic cracking represents a promising approach, as it operates under mild temperature and pressure conditions without relying on external hydrogen supply or noble-metal catalysts. Microporous zeolites are widely employed in the catalytic cracking of biomass- [2] and plastic-derived [3] pyrolysis vapors due to their peculiar pore structure and strong Brønsted acidity. Olive stone is an abundant lignocellulosic residue in the Mediterranean area, with approximately one ton generated per ton of olive oil produced [4]. In this study, olive stone valorization was investigated via an ex-situ catalytic fast pyrolysis (CFP) process, with specific focus on the coke-induced deactivation mechanisms of a commercial HZSM-5 zeolite catalyst (TOSOH Chemicals, Tokyo, Japan). Thermal pyrolysis was conducted in a spouted-bed reactor, characterized by intense gas–solid contact and enhanced heat and mass transfer rates, followed by downstream catalytic upgrading in a fixed-bed reactor. Fresh and spent catalysts, collected after continuous operation under different reaction conditions, were systematically characterized. Textural properties were determined by N_2 adsorption–desorption cycles at 77 K (BET and BHJ methods), total acidity was quantified by NH_3 temperature-programmed desorption (NH_3-TPD), and coke content and speciation were evaluated by temperature-programmed oxidation (TPO). Results revealed rapid catalyst deactivation after only 45 min of continuous operation, with coke deposition reaching approximately 10 wt% and a substantial decrease in specific surface area and pore volume. The marked loss of accessible acid sites and pore blockage highlights the critical impact of coke formation on catalytic performance, emphasizing the need for improved formulations and regeneration strategies to enhance catalyst stability under biomass CFP conditions.

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