
XII ENCMP
Universidade de Coimbra
6-7 Junho 2024
XII Encontro Nacional de Catálise e Materiais Porosos
1 2 9 0 UNIVERSIDADE D COIMBRA
SOCIEDADE PORTUGUESA DE QUÍMICA

Bem-vindos ao XII ENCMP

É com grande prazer que damos as boas-vindas a todos os participantes ao **XII Encontro da Divisão de Catálise e Materiais Porosos da Sociedade Portuguesa de Química!!**

A divisão foi criada em 1992, durante o Congresso Nacional da Sociedade Portuguesa de Química, em Lisboa. Esse foi o início da reação, tendo esta sido catalisada com base no estímulo da colaboração entre os diferentes grupos de investigação de catálise e materiais existentes nas diversas universidades portuguesas, e garantir a organização de um encontro científico bienal. Em 1993 organizava-se então, na Universidade de Aveiro, o 1º Encontro da Divisão de Catálise da SPQ. À época, reuniu 54 participantes de 18 grupos de investigação das várias universidades e institutos superiores Portugueses. Se naquela altura a investigação em catálise heterogénea era predominante, hoje, 30 anos volvidos, estamos reunidos em Coimbra para iniciar o *XII Encontro de Catálise e Materiais Porosos*, com cerca de 100 participantes de todas as universidades e centros de investigação de Portugal, abrangendo todos os domínios da catálise: heterogénea, homogénea, eletrocatalítica e biocatalítica.

O Grupo de Catálise & Química Fina da Universidade de Coimbra, fundado em 2000, tem sido um participante ativo nas atividades desta divisão. Em 2007, organizou o 8º Encontro da Divisão de Catálise e Materiais Porosos da SPQ, realizado em Lamego e o Curso InterUniversitário de Catálise. Além disso, em 2015, foi responsável por sediar o Encontro Ibero-Americano de Catálise, em simultâneo com o Encontro Nacional de Catálise e Materiais Porosos, que contou com a participação de mais de 450 cientistas.

Em 2024, temos o prazer de receber novamente, em Coimbra, a comunidade de investigadores em catálise. Este encontro ultrapassa as fronteiras portuguesas, com conferencistas de Espanha, Hungria, Inglaterra e Brasil. Sendo a catálise um ramo da ciência naturalmente agregador e multidisciplinar, esperamos que deste encontro surjam novas ideias e colaborações, contribuindo para o crescimento da comunidade de catálise em Portugal e no mundo. Este crescimento também é sinónimo de desenvolvimento económico do país.

Neste livro do *XII Encontro da Divisão de Catálise e Materiais Porosos*, apresentam-se os resumos de 4 lições plenárias convidadas, de 9 keynotes, de 35 comunicações orais e de 22 comunicações em poster.

A Comissão Organizadora do *XII Encontro de Catálise e Materiais Porosos* deseja a todos os colegas e amigos dois inesquecíveis dias em Coimbra, que para além das frutíferas discussões científicas, irá culminar com a participação na “Workshop de Biocatálise” na PRAXIS de Coimbra, dia 6 de junho.

À medida que avançamos para o futuro, é certo que a ciência, e especialmente a catálise, continuarão a progredir com o auxílio da inteligência artificial. Encerramos com um poema da autoria do Chat GPT dedicado aos catalíticos hoje reunidos em Coimbra:

Neste encontro de mentes brilhantes,
Em Coimbra, onde a ciência se levanta,
A catálise é a estrela que brilha,
Na dança das moléculas em maravilha.

Na lira subtil das moléculas em dança,
Onde o tempo desliza, a ciência se lança,
Surge a catálise, que poupa tempo e energia,
Nas reações químicas, uma nobre sinfonia.

Um sussurro suave na química dos seres,
Que desata os nós, quebra barreiras,
Catalisador, és tu o segredo oculto,
Do simples ao complexo, fazes salto de vulto

Com a inteligência artificial a guiar,
Novos horizontes iremos desbravar,
Catalisadores, heróis da reação,
Que impulsionam a inovação com paixão.

Que este encontro seja fonte de inspiração,
Para novas descobertas em profusão,
E que a catálise, com seu poder,
Continue a nos surpreender e a crescer.

Coimbra, 6 e 7 de junho de 2024
Saudações académicas

P'la Comissão Organizadora
Mariette Pereira
Mário Calvete

SOCIEDADE PORTUGUESA DE QUÍMICA

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Welcome to the XII ENCMP

It is with great pleasure that we welcome all participants to the **XII Meeting of the Catalysis and Porous Materials Division of the Portuguese Chemical Society**!!

The division was created in 1992 during the National Congress of the Portuguese Chemical Society in Lisbon. That was the beginning of the reaction, which was catalyzed by encouraging collaboration between the different catalysis and materials research groups at the various Portuguese universities, and ensuring the organization of a biennial scientific meeting. In 1993, the 1st Meeting of the Catalysis Division of the SPQ was organized at the University of Aveiro. At the time, it brought together 54 participants from 18 research groups from various Portuguese universities and colleges. While at that time research into heterogeneous catalysis was predominant, today, 30 years later, we are gathered in Coimbra to start the XII Meeting on Catalysis and Porous Materials, with around 100 participants from all the universities and research centers in Portugal, covering all the fields of catalysis: heterogeneous, homogeneous, electrocatalytic and biocatalytic.

The Catalysis & Fine Chemistry Group of the University of Coimbra, founded in 2000, has been an active participant in the division's activities. In 2007, it organized the 8th Meeting of the Catalysis and Porous Materials Division of the SPQ, held in Lamego, and the Inter-University Course on Catalysis. In addition, in 2015, it was responsible for hosting the Ibero-American Catalysis Meeting, at the same time as the National Catalysis and Porous Materials Meeting, which was attended by more than 450 scientists.

In 2024, we are pleased to welcome the community of catalysis researchers to Coimbra once again. This meeting goes beyond Portuguese borders, with speakers from Spain, Hungary, England and Brazil. Since catalysis is a naturally aggregating and multidisciplinary branch of science, we hope that new ideas and collaborations will emerge from this meeting, contributing to the growth of the catalysis community in Portugal and around the world. This growth is also synonymous with the country's economic development.

This book of the XII Meeting of the Catalysis and Porous Materials Division presents the abstracts of 4 invited plenary lectures, 9 keynotes, 35 oral communications and 22 poster communications, as well as the Ramôa Ribeiro awards for the Best Thesis in Catalysis and Porous Materials and for the Best Young Researcher in Catalysis and Porous Materials.

The Organizing Committee of the XII Meeting on Catalysis and Porous Materials wishes all colleagues and friends two unforgettable days in Coimbra, which, in addition to fruitful scientific discussions, will culminate with participation in the “Biocatalysis Workshop” at PRAXIS in Coimbra on June 6.

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Local do Encontro/Venue

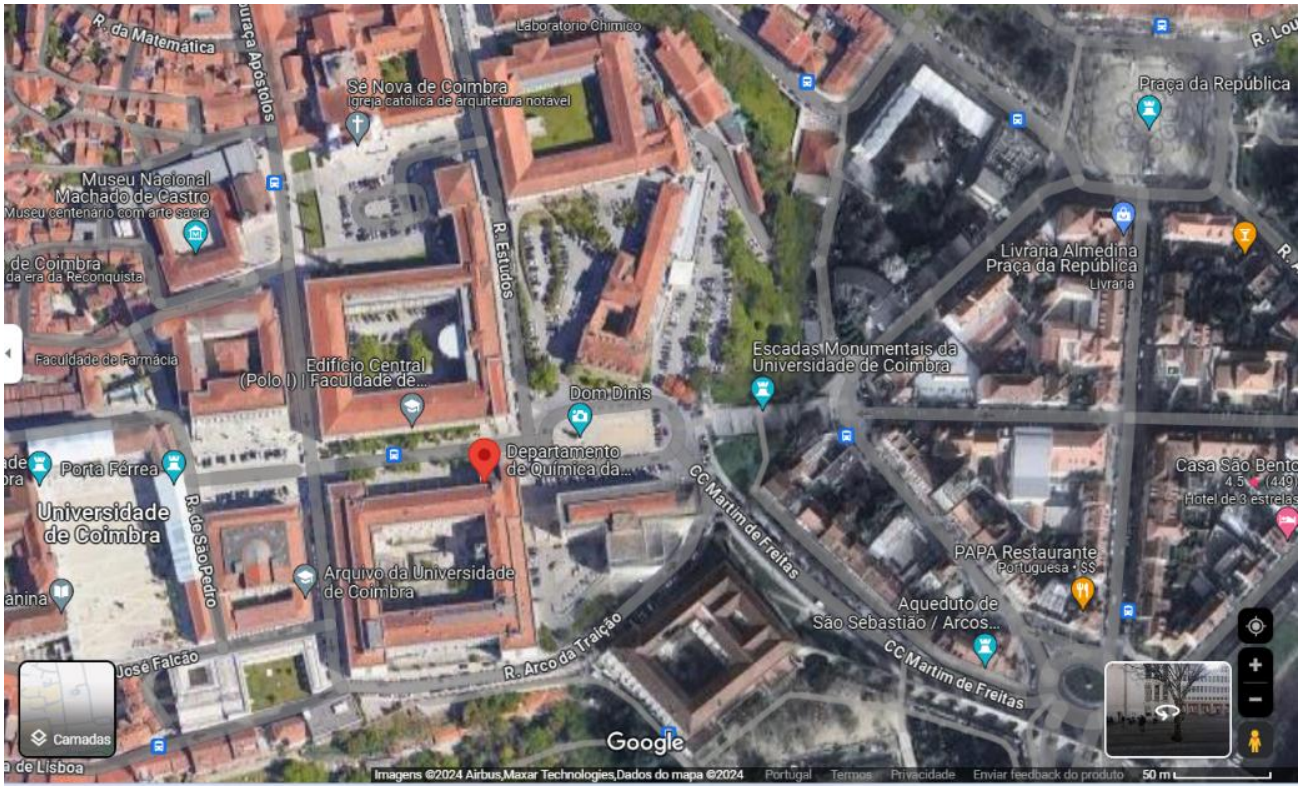
O Encontro realiza-se no Departamento de Química da Faculdade de Ciências e Tecnologia da Universidade de Coimbra.

The Meeting takes place at the Department of Chemistry of the Faculty of Sciences and Technology of the University of Coimbra.

Morada/address

Polo I - Departamento de Química, Rua Larga, 3004-535, Coimbra

Coordenadas GPS (Latitude: 40.207925 | Longitude: -8.423696)



XII ENCMP 2024, 6-7 June 2024

PROGRAM OVERVIEW

Thursday, 6 June 2024	
10.00 – 10.45	**Reception desk**
10.45 – 11.00 Auditorium	**Welcome & Introduction**
Session 1	Chair (Auditorium): *José L. Figueiredo/Luísa M. Martins*
11.00 – 11.40	PL1: "Exploring the pore space of transition metal- and Ln-silicates, and MOFs" João Rocha – Univ. Aveiro
11.40 – 12.00	KN1: "Interfacing photosynthetic biomolecules with electrodes for light-driven H_2 production" Felipe Conzuelo – ITQB Univ. Nova Lisboa
12.00 – 12.20	KN2: "Harnessing visible light for cleaner water and sustainable chemical and fuels" Maria Sampaio – Univ. Porto
12.20 – 14.00	LUNCH BREAK
Session 2	Chair (Auditorium): *Joaquim Faria/Marta Piñeiro*
14.00 – 14.40	PL2: "Activation of molecular oxygen and selective oxidation" Janliang Xiao – Univ. Liverpool, UK
14.40 – 15.00	KN3: "Empowering biomass wastes through catalysis: Sustainable synthesis of high-value chemicals and fuels" Lucília Ribeiro – Univ. Porto
15.00 – 15.20	OP1: Prémio melhor tese de Doutoramento em Catálise e Materiais Porosos – André Torres Pinto – Univ. Porto
15.20 – 15.30	OC1: "Depolymerization of plastic waste catalyzed by homogeneous and heterogeneous catalysts" Ana Fernandes – IST Univ. Lisboa
15.30 – 15.40	OC2: "Transformation of biomass model compounds using Pt-Ni/Y catalyst prepared by mechanochemistry" Mariana Matos – , ISEL – Inst. Politécnico de Lisboa
15.40 – 15.50	OC3: "Cork-derived activated carbon for environmentally friendly supercapacitors" Raquel Rocha – Univ. Porto
15.50 – 16.00	OC4: "From Combustion Residues to magnetic catalysts: Innovative tool for water pollutant valorization" Iwona Kuźniarska-Biernacka – Univ. Porto
16.00 – 16.10	Q&A
16.00 – 17.00	Coffee break & Poster Session
Session 3	Chair (Auditorium): *Ana Paula Carvalho/Isabel Correia Neves*
17.00 – 17.20	KN4: "Catalytic valorization of biomass-derived synthons" Rafael Gomes – Univ. Lisboa, Portugal
17.20 – 17.30	OC5: "Ethylene photocatalytic oxidation for fruit ripening mitigation using TiO2-based zeolite materials" Ricardo Ferreira – IST Univ. Lisboa
17.30 – 17.40	OC6: "Crude glycerol: using acid zeolites to obtain fuel additives" Isabel Santos-Vieira – Univ. Aveiro
17.40 – 17.45	Q&A
17.45 – 18.45	Catalysis and Porous Materials Division (DCMP) Meeting – **open to all members (in Classroom C16)**
19:00 – 19:30	Experimental workshop 1 : Biocatalysis – Producing liquids that you can drink!
19:30 – 20:00	Experimental workshop 2 : Biocatalysis – Producing liquids that you can drink!
20:00 – 20:30	Experimental workshop 3 : Biocatalysis – Producing liquids that you can drink!
20.30	Galla Dinner - at PRAXIS (Coimbra)

Friday Morning, 7 June 2024		
Session 4	Chair (Auditorium):*Cristina Freire/Beatriz Royo*	
9.00 – 9.40	PL3: "Synergistic approaches to catalyst design: from benchmark to elusive substrates" Montserrat Diéguez – Univ Rovira I Virgili, Spain	
9.40 – 10.00	KN5: "Functionalized metal–organic frameworks as platforms for gas adsorption and catalysis" Anirban Karmakar – IST Univ. Lisboa	
	Chair (Auditorium): *Cristina Freire/Beatriz Royo*	Chair (Classroom): *Andreia Peixoto/Sara M. Pinto*
10.00 – 10.10	OC7: "Mechanochemistry and catalysis, a powerful alliance for the development of sustainable processes" Marta Piñeiro – Univ. Coimbra	OC23: "Optimizing drug combinations for melanoma therapy by machine learning in zeolite delivery systems" Ana Raquel Bertão – Univ. Minho
10.10 – 10.20	OC8: "Biodiesel additives synthesis using metal(IV) phosphates catalysts: Esterification of levulinic acid" Graça Rocha – Univ. Aveiro	OC24: "Biomass-derived catalysts: heteroatom doping and metal incorporation towards high performance oxygen reduction" Renata Matos – Univ. Porto
10.20 – 10.30	OC9: "Sustainable fuel desulfurization using advanced porous catalytic membranes" Rui Faria – Univ. Porto	OC25: "Development of waste-based carbon dots as photo-nanocatalysts" Luís Silva – Univ. Porto
10.30 – 10.40	OC10: "Chlorophyll as a natural photocatalyst to obtain antimicrobial compounds from rosin oxidation" Cláudia Neves – Inst. Politécnico de Viseu	OC26: "Pd-catalyzed aminocarbonylation continuous-flow process: Multigram synthesis of carboxamides" Fabio Rodrigues – Univ. Coimbra
10.40 – 10.50	Q&A	Q&A
10.50– 11:15	Coffee break & Poster Session	
Session 5	Chair (Auditorium): *M. Graça Neves/Helder Gomes*	
11.15 – 11.35	KN6: "Sustainable Catalytic Processes for CO_2 Valorization" Rui Carrilho – Univ. Coimbra	
11.35 – 11.55	KN7: "C–N bonding formation mediated by transition metals: a useful tool to modify the porphyrin core" Nuno Moura – Univ. Aveiro	
	Chair (Auditorium): *M. Graça Neves/Helder Gomes*	Chair (Classroom): *Fábio Rodrigues/Rafael Aroso*
11.55 – 12.05	OC11: "Rapid formation of vinylene linked phenanthroline covalent organic frameworks for photocatalysis" Clara Ponte – International Iberian Nanotechnology Laboratory, Braga	OC27: "Highly selective phthalocyanine-based catalysts for CO2 addition reactions to epoxides" Andreia Gonzalez – Univ. Coimbra
12.05 – 12.15	OC12: "Green aromatic epoxidation with an iron porphyrin catalyst for functionalization of renewable xylene, quinoline, and acridine" Gabriela Corrêa – Univ. Porto	OC28: "Tröger's base–linked POPs as heterogeneous catalysts for the nitroaldol condensation" Tiago Machado – Univ. Coimbra
12.15 – 12.25	OC13: "Sustainable approaches for CO2 catalytic conversion into fuels and valuable products" Luís Branco – Univ. Nova Lisboa	OC29: "Upgrading of biomass derivatives to biobased products for drop-in-fuels and chemicals over Niobium-based catalysts" Margarida Antunes – Univ. Aveiro
12.25 – 12.35	Q&A	Q&A
12.35– 14.00	LUNCH BREAK	

Friday Afternoon, 7 June 2024		
Session 6	Chair (Auditorium): *José Cavaleiro/Filipa Ribeiro*	
14.00 – 14.40	PL4: "Photocatalyzed and electrochemical reactions in both batch and continuous flow conditions: recent applications for fine chemicals and API's synthesis" Kleber T. Oliveira, Univ. S. Carlos, Brasil	
14.40 – 15.00	KN8: "Carbon nanotubes derived from plastic solid waste: catalytic applications" Helder Gomes – Inst. Politécnico de Bragança	
15.00 – 15.25	OP2: Prémio Ramôa Ribeiro investigador jovem – Mirtha Lourenço – Univ. Aveiro	
	Chair (Auditorium): *José Cavaleiro/Filipa Ribeiro*	Chair (Classroom): *Rui Carrilho/Andreia Peixoto*
15.25 – 15.35	OC14: "Synthesis of functional polymers for selective adsorption of bioactive compounds from olive leaf extracts" Ayssata Almeida – Inst. Politécnico de Bragança	OC30: "Fruit ripening mitigation – Ag-based-ZSM-5 materials for ethylene removal under competitive adsorption" Lívia Valle, – IST Univ. Lisboa
15.35 – 15.45	OC15: "Advanced smart textiles: Electrochromic supercapacitors boosted by glucose-derived carbon and PEDOT:PSS" Gabriela Queiroz – Univ. Porto	OC31: "Advanced heterogeneous degradation strategies for trimethoprim using porphyrin catalysts: From H2O2 treatment to photocatalysis and flow chemistry processes" Giusi Piccirillo – Univ. Coimbra
15.45 – 15.55	OC16: "Polyoxotungstates@MIL-100(Fe) to achieve sustainable oxidative desulfurization and denitrogenation of fuels" Diniz Silva – Univ. Porto	OC32: "Getting Insights about zeolite desilication through machine Learning" Daniel Costa – IST Univ. Lisboa
15.55 – 16.05	OC17: "Construction of a sustainable photocatalytic solar reactor: study of the degradation of indigo carmine blue food coloring" Fernando Pereira de Sá, Instituto Federal de Educação, Ciência e Tecnologia de Goiás, Brasil	OC33: "Improved ethylene production over Calcium doped LaInO3 perovskite nanofibers" Joana Martinho – IST Univ. Lisboa
16.05 – 16.15	Q&A	Q&A
16.15 – 16.30	Coffee break	
Session 7	Chair (Auditorium): *Mariette Pereira/Mário Calvete*	
16.30 – 16.50	KN9: "Functional porous materials for energy and biomedical applications" Sandra Gago – Univ. Nova Lisboa	
16.50 – 17.00	OC18: "Synthesis of 2-methylresorcinol-based cavitands by means of homogeneous catalytic reactions" László Kollar – Univ. Pécs, Hungria	
17.00 – 17.10	OC19: "Porous MOF-based materials with high potential to sustainable catalytic processes" Luís Cunha-Silva – Univ. Porto	
17.10 – 17.20	OC20: "Nanostructured binuclear catalysts and nanozymes by ionic self-assembly of first-row transition metalloporphyrins" Susana Rebelo – Univ. Porto,	
17.20 – 17.30	OC21: "CO oxidation on single-atom catalysts based on the molybdenum carbide (Mo2CO2) MXene" José Gouveia – Univ. Aveiro	
17.30 – 17.40	OC22: "Catalytic system for conversion of sugarcane molasses waste to 5-hydroxymethylfurfural" Katarzyna Eblagon – Univ. Porto	
17.40 – 17.50	Q&A	
17.50 – 18.15	Closing session and Best Poster Award	

Comunicações Científicas/Scientific Contributions

PLENARY LECTURE ABSTRACTS

PL 1

Exploring the pore space of transition metal- and Ln-silicates, and MOFs

João Rocha[a,*]

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Scientific topic: Preparation of new catalysts and/or porous materials

Zeolites are porous, crystalline aluminosilicates with frameworks built from tetrahedral units connected by oxygen atoms, featuring exchangeable cations. They are used in catalysis, gas separation, and ion-exchange. Beyond zeolites, certain microporous silicates are assembled from transition-metal and lanthanide bearing heteropolyhedra and, in addition to the conventional zeolite properties, they exhibit magnetism and light emission. This talk presents examples of applications of such materials developed in my laboratory in light emission devices[1] and in the treatment of the medical condition hyperkalemia (excess K^+ in serum), with a new drug now on the market.[2]

Metal Organic Frameworks (MOFs) are hybrid materials with polyatomic metal clusters linked by covalent bonds to form nanoporous structures. In contrast with zeolitic materials, MOFs operate in milder conditions and, comparatively, often lack robustness, but they are much more amenable to 'rational synthesis' and post-synthetic modification using the conventional methods of organic synthesis. In this talk, I shall present some examples of my groups' research on MOFs, encompassing temperature sensing via light emission,[3] anti-mosquito textile nets, and uranyl ion capture from waters.[4] Moreover, I will highlight some of our recent efforts to design: (i) efficient electrically conductive MOFs based on the partially oxidised perylene ligand, aiming at applications in (opto)electronics, electrocatalysis and energy storage, among others;[5] (ii) luminescent MOFs based on persistent neutral organic (e.g., triphenylmethyl) radicals that also present magnetic and electrochemical properties.[6]

Acknowledgements
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PL 2

Activation of molecular oxygen and selective oxidation

Janliang Xiao

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Scientific topic: Preparation of new catalysts and/or porous materials; Photocatalysis

Molecular oxygen is indispensable to life, playing essential roles in many life-dependent chemical reactions. Whilst nature has mastered the mechanism of how to harness the reactions of O_2, activation and use of O_2 for selective oxidation remain challenging for chemist. This lecture will introduce some of the work we have been doing on selective oxidation by O_2 using catalysts based on earth-abundant, bio-benign metals.[1-6]

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PL 3

Synergistic approaches to catalyst design: from benchmark to elusive substrates

Montserrat Diéguez*, M. Biosca, M. A. Pericàs and O. Pamiès

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Scientific topic: Homogeneous catalysis

Developments in the synthesis of chiral molecules, whether producing new compounds or improving current synthetic procedures, are made possible by constant innovations in asymmetric catalysis. To fully exploit the application of asymmetric catalysis, there is a continuous necessity to expand the range of substrates undergoing the process with high enantioselectivity, thus making the preparation of the most diverse chiral molecules possible. The finding of a catalyst that could work for new substrate types is hampered because of the lack of data, since most of the catalytic systems have only been tested using benchmark substrates. In order to limit time-consuming catalyst design is highly desirable to identify catalyst with a broad substrate scope.

So, in this context I will present several examples that will illustrate different ways to integrate theoretical calculations into the catalyst design (from guiding it to predictive models going through in silico-based catalyst optimization) for the synthesis of elusive chiral synthons. Special attention will be paid to recent examples involving several asymmetric transformations.[1] I will also discuss how to improve the chemical sustainability of the process with the development of continuous flow versions by using immobilized versions of the catalysts.

Acknowledgements
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PL4

Photocatalyzed and electrochemical reactions in both batch and continuous flow conditions: recent applications for fine chemicals and API's synthesis

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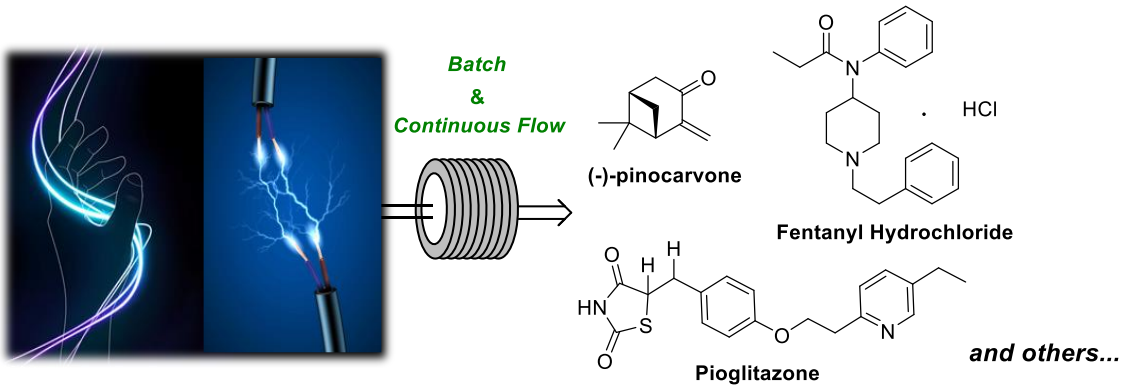
Scientific topic: Photocatalysis

Recent literature has placed a renewed focus on photocatalyzed and electrochemical reactions, recognizing their pivotal role in advancing sustainable organic transformations and their scalability.[1-3] These reactions, coupled with enabling technologies like continuous flow conditions, have been strategically utilized to synthesize fine chemicals and active pharmaceutical ingredients (APIs).[4] The integration of these innovative techniques has significantly enhanced the efficiency, sustainability, and safety of thermal, photo, and electrochemical reactions in producing key molecules.[5] In this presentation, the impact of flow chemistry on the synthesis of fine chemicals and APIs, particularly when leveraged alongside photocatalyzed and electrochemical reactions will be covered showing some methodologies and applications in synthesizing important molecules such as pinocarvone, fentanyl (an anesthetic), pioglitazone, and others.



Scheme or Figure 1: Flow Chemistry for Fine Chemicals and API's Synthesis.

Acknowledgments

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PRIZE PRESENTATION ABSTRACTS

OP1

Best PhD thesis in Catalysis and Porous Materials Award

Optimised 2D carbon materials activated by artificial light and electrical current for catalytic water and wastewater treatment

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Scientific topic: Photocatalysis

The development of sustainable water treatment technologies is crucial to obtain clean water. For this reason, heterogeneous advanced oxidation processes with graphitic carbon nitride (herein designated as g-C_3N_4 or GCN) can be presented as a promising solution. GCN is a well-known photocatalyst that can be activated by visible-light irradiation. However, it is necessary to optimise the synthesis process to improve its catalytic activity, appropriately tuning the resulting physicochemical properties. Nanostructured GCN materials were synthesised and modified by thermal exfoliation, precursor selection and chemical functionalisation, demonstrating that the most promising catalyst was achieved by direct thermal polymerisation of urea [1].
In the presence of certain molecules (organic contaminants), GCN can lead to the formation and consequent activation of hydrogen peroxide (H_2O_2), accelerating the degradation process and obtaining a proven self-sufficient technology in the treatment of waters rich in phenolic compounds, present in agro-industrial effluents [2, 3].
The photo-electrocatalytic application of GCN (simultaneous activation by light irradiation and electrical current) was also investigated, allowing greater performance than under the influence of light alone. This technology was used to remove pharmaceutical compounds, typically present in urban wastewaters [4].
The work resulted in the creation of a photo-electrocatalytic system with high efficiency in removing organic compounds from real water, capable of scalability and integration with other technologies.

Acknowledgements
This work was supported by FCT/MCTES (PIDDAC) under project DRopH2O - 2022.08738.PTDC (DOI: 10.54499/2022.08738.PTDC). This research was also funded by FCT/MCTES (PIDDAC) under projects: SuN2Fuel - 2022.04682.PTDC (DOI: 10.54499/2022.04682.PTDC), LSRE-LCM, UIDB/50020/2020 (DOI: 10.54499/UIDB/50020/2020) and UIDP/50020/2020 (DOI: 10.54499/UIDP/50020/2020); and ALiCE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020).

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OP2

Ramôa Ribeiro Young Resercher Award

Advancing porous materials design for CO_2 capture

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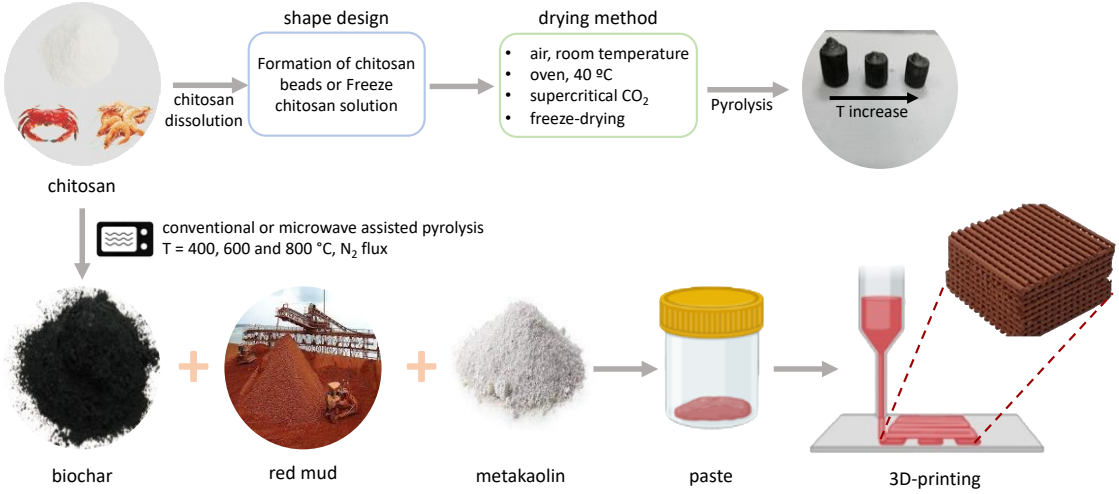
Scientific topic: Porous materials for energy and environment

CO_2 adsorption technology is recognized as a highly effective method for reducing greenhouse gas emissions. Biochars emerge as promising CO_2 adsorbents, offering customizable properties and sustainable production by adjusting pyrolysis conditions and biowaste feedstocks.[1]
Our work focused on advancing CO_2 capture technologies by designing biochar adsorbents derived from chitosan, employing innovative approaches to enhance adsorption efficiency. By using advanced characterization techniques, including XPS, gas sorption isotherms, electron microscopy, and operando TGA-IR, we aim to gain a comprehensive molecular-level understanding of biochar microstructure and CO_2 adsorption mechanisms.
We investigated how polymerization, drying methods, heating techniques, and pyrolysis temperatures affect the textural properties and adsorption behavior of biochars derived from chitosan. Furthermore, we explored the potential of a 3D-printed biochar composite with inorganic polymers (Scheme 1). Our findings showcased the effectiveness of biochar in CO_2 adsorption applications, particularly for CO_2/CH_4 and CO_2/N_2 separation under both dry and moist conditions.
By designing powder and self-standing N-doped biochar adsorbents with varying textural properties, we identified correlations between microstructure and CO_2 adsorption efficiency. These moisture-tolerant materials, dominated by physisorption, seem to be suitable for cyclic separation processes. The sustainable production of biochar, achieved without additional activation or functionalization steps, along with their self-standing configurations, positions these residue-derived adsorbents as highly promising for large-scale CO_2 separation applications.



Scheme 1: Illustration of the synthesis protocols for biochars-derived sorbents.

Acknowledgements
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KEYNOTE PRESENTATION ABSTRACTS

KN1

Interfacing photosynthetic biomolecules with electrodes for light-driven H_2 production

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Scientific topic: Biocatalysis

Oxygenic photosynthesis is perhaps one of the most important natural processes sustaining life on Earth through the production of molecular oxygen and the assimilation of carbon dioxide into organic matter. The process is driven by the absorption of sunlight as the primary energy source and relies on two sequential photoinduced charge separation steps performed by the membrane-protein complexes known as photosystem I (PSI) and photosystem II (PSII). The photosynthetic protein complexes are highly abundant in nature and have an exceptionally high quantum yield, close to 100%, for the photon-to-electron conversion. As a result, there is a great interest in the coupling of these biomolecules with electrode materials for the development of semi-artificial biodevices that will enable the conversion of solar light energy into electrical power as well as the synthesis of valuable products. In particular, PSI is of great interest as a building block for the fabrication of bio-hybrid solar energy conversion devices. Resembling a photodiode, PSI is able to pump electrons to a high energy level upon absorption of visible light. After subsequent internal electron transfer, a relatively long-lived state is obtained consisting of two redox centers of opposite charge with a potential difference of about one volt. On this basis, PSI can be exploited for the fabrication of photocatalytic electrodes performing reduction reactions of interest. However, the considerably large voltage difference between the two opposite redox sites at PSI translates directly into a substantial driving force for recombination processes and the re-oxidation of reduced charge carriers at the electrode surface, thus canceling out part of the generated photocurrents and compromising the efficiency of the fabricated biophotovoltaic devices.[1] Therefore, one of the major challenges in the development of PSI-based devices constitutes the fabrication of well-defined structures able to provide a unidirectional electron flow. As it will be shown, a rational integration of PSI with redox mediators and (bio)catalysts performing H_2 evolution allows the efficient transfer of high-energy electrons generated upon the absorption of visible light to the catalyst for the reduction of protons in solution.[2-4]

Acknowledgements
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KN2

Harnessing visible light for cleaner water and sustainable chemical and fuels

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Scientific topic: Photocatalysis

In response to the growing demand for clean water, sustainable energy, and eco-friendly chemicals, the scientific and industrial communities are being actively exploring the potential of artificial photosynthesis to harness sunlight as energy source. Heterogeneous photocatalysis reactions driven by semiconductor nanomaterials are becoming increasingly significant for process intensification and safety in a variety of applications, particularly in the domains of water treatment, energy production, and organic synthesis. The key for the implementation of such technology lies in the successful combination of energy-efficient irradiation, effective and sustainable catalysts, and appropriate reactor engineering. Despite the efficiency of photocatalysts (*e.g.*, TiO_2, WO_3, ZnO) in various applications [1], graphitic carbon nitride (g-C_3N_4) has particularly revealed great potential under visible light (bandgap energy ~2.7 eV). The remarkable physicochemical stability, and the abundance of "earth-abundant" elements such as C, N, and H, makes g-C_3N_4 as an excellent candidate for solar-driven photocatalytic applications [2-4]. Nevertheless, challenges remain in this field, particularly when the catalysts are employed in powder form, which include the catalyst's difficult separation, particle aggregation, and complications in implementing the technology in continuous flow processes. This talk will present approaches for boosting the activity of g-C_3N_4 in distinct photocatalytic applications ranging from hydrogen (H_2) and hydrogen peroxide (H_2O_2) production, chemical synthesis, and water treatment (Figure 1). The use of such materials immobilized in different supports will also be discussed.

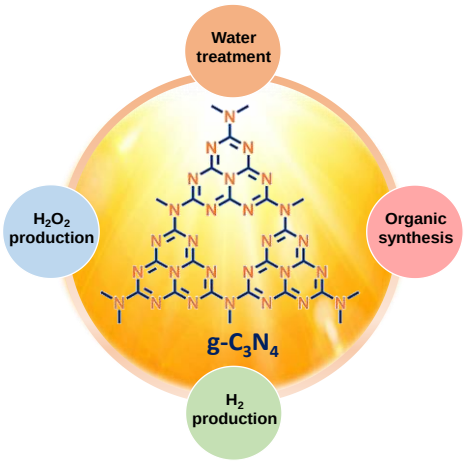

Figure 1. Photocatalytic applications of g-C_3N_4.

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KN3

Empowering biomass wastes through catalysis: Sustainable synthesis of high-value chemicals and fuels

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Scientific topic: Heterogeneous catalysis

Biomass is any hydrocarbon that mainly consists of carbon, hydrogen, oxygen and nitrogen, and is mainly composed of cellulose, hemicelluloses and lignin.[1] The catalytic valorization of biomass wastes is a promising technology that can link the traditional refinery and renewable sources. Considering the availability of forestry and agricultural feedstocks, aquatic plants and algae, as well as municipal and industrial wastes, there is a great worldwide potential for the production of highly valuable chemicals and fuels from biomass. For example, sorbitol and ethylene glycol (EG) are extremely important chemicals that are extensively used in food, pharmaceutical, and chemical industries. Great progress was obtained in their selective production over a variety of highly efficient heterogeneous catalysts.

The conversion of cellulose into sorbitol was studied by coupling hydrolysis of cellulose to glucose and its subsequent hydrogenation. Sorbitol yields up to 70 and 48 % were attained from the one-pot conversion of cellulose and cellulosic wastes (e.g., tissue paper, cotton wool, cotton textile), respectively, over carbon nanotubes (CNT) supported Ru catalysts.[2] Then, Ru catalysts supported on glucose-derived carbons were synthesized, allowing to achieve a remarkable 100 % conversion of cellulose with a sorbitol yield of 64 % in just 3 h, which outstood previous results.[3]

Alternatively, Ru–W bimetallic catalysts supported on glucose-derived carbons were used for the direct conversion of cellulose to EG, allowing to achieve yields close to 50 % in just 3 h.[4] Furthermore, CNT-supported Ru-W catalysts were tested for the production of EG from various forestry, agricultural and urban wastes, such as woods (pine, oak, eucalyptus, etc.), leaves (eucalyptus, lemon), pine cones, cork, corncob, grass, flowers, peanut shells, coffee grounds, cotton wool and paper. The highest yields could be directly obtained from eucalyptus wood and cotton wool (41 %).[5] More recently, a cheaper metal such as Ni was found to successfully replace the Ru noble metal for cellulose conversion into EG. [6] An EG yield over 50 % was reached in just 5 h over Ni-W/CNT, which greatly surpassed the previous obtained using Ru-W/CNT. Additionally, the catalyst was tested for the conversion of cotton wool, eucalyptus wood and corncob, resulting in EG yields of 43, 28 and 36 %, respectively.[6]

These results are very encouraging for large scale applications, and the accumulated knowledge from these extensive studies will be a valuable guide for tuning the reaction selectivity and meeting the market demand.

Acknowledgements
This work was supported by national funds through FCT/MCTES (PIDDAC): LSRE-LCM, UIDB/50020/2020 (DOI: 10.54499/UIDB/50020/2020) and UIDP/50020/2020 (DOI: 10.54499/UIDP/50020/2020); ALiCE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020).

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KN4

Catalytic valorization of biomass-derived synthons

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Scientific topic: Heterogeneous catalysis

The preparation of both bulk and fine chemicals has seen a paradigm change towards sustainability. Whether it be the development of catalytic procedures over stoichiometric ones, replacing hazardous solvents or the use of renewable raw materials. In compliance with the 12 principles of green chemistry, lignocellulosic biomass has been used as source of synthons for the preparation of chemical commodities, fuels and fine chemicals.

We and several others have been involved in the development of catalytic methodologies for the upgrading of biomass derived synthons. Here we showcase some of our efforts to obtain valuable molecules from simple furanic biorenewables, namely the obtention of trans-4,5-diaminocyclopentenones;[1] the total synthesis of a cytotoxic natural product, Agelastatin A, from the catalytic upgrading of furfural;[2] and cascade reactions such as Diels-Alder/aromatization catalytic systems for the preparation of commodity chemicals.[3] In addition we extend our scope of biorenewables towards chitinous biomass[4] and olive leaves crude extracts,[5] by employing heterogeneous acid catalysts in order to obtain valuable fine chemicals.

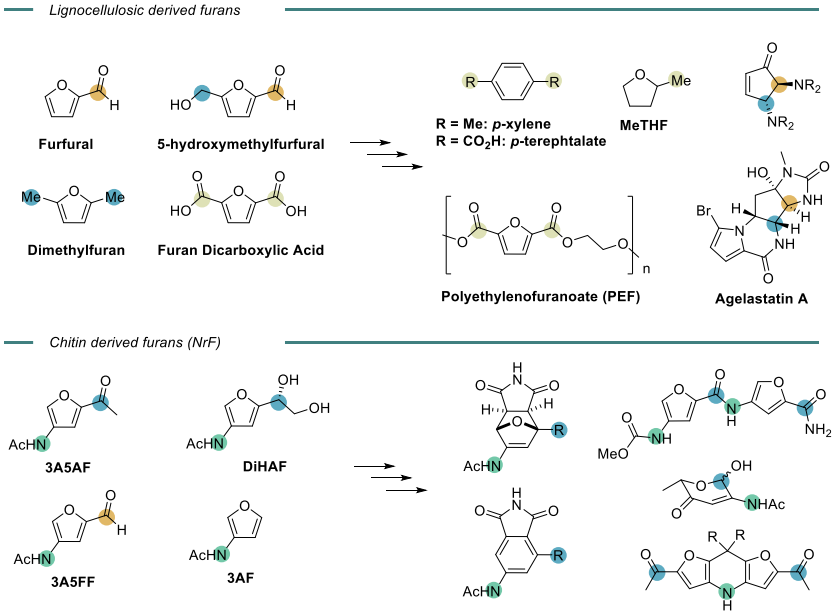

Figure 1: Selected transformations of biomass furanics

Acknowledgements
The authors acknowledge Fundação para a Ciência e Tecnologia (FCT) for financial support (PTDC/QUI-QOR/32008/2017, UIDB/04138/2020, UIDP/04138/2020, PTDC/MED-QUI/1947/2020 and PTDC/QUI-OUT/3989/2021). The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 951996.

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KN5

Functionalized Metal–organic frameworks as platforms for gas adsorption and catalysis

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Scientific topic: Porous materials for energy and environment

Abstract
Metal–organic frameworks (MOFs) are crystalline coordination networks consisting of metal ions or clusters and multidentate organic ligands[1]. This area of research is currently undergoing a rapid growth due to their potential applications as functional materials in heterogeneous catalysis, magnetism, nonlinear optics, gas storage and separation, etc[2]. Moreover, MOFs constructed from functionalized linkers have attracted considerable attention due to their interesting topologies, gas adsorption and catalytic properties[3]. Thus, we have synthesized various halogen and thiophene functionalized multifunctional carboxylate ligands and employed them for the construction of various three-dimensional MOFs. These MOFs were characterized by X-ray single crystal diffraction, elemental microanalysis, FT-IR spectroscopy, thermogravimetric analysis and powder X-ray diffraction analysis. The gas adsorption analysis of these MOFs demonstrate that they display high uptake of CO_2 (up to 5.34 mmol/g) over N_2 and CH_4[4]. In order to understand the mechanism behind the better adsorption of CO_2 by our MOFs we have also performed configurational bias Monte Carlo simulation studies. Moreover, due to the presence of Lewis acidic metal centers these MOFs act as heterogeneous catalysts for the CO_2 fixation reactions with different epoxides in the presence of tetrabutyl ammonium bromide (TBAB), for conversion into industrially valuable cyclic carbonates.

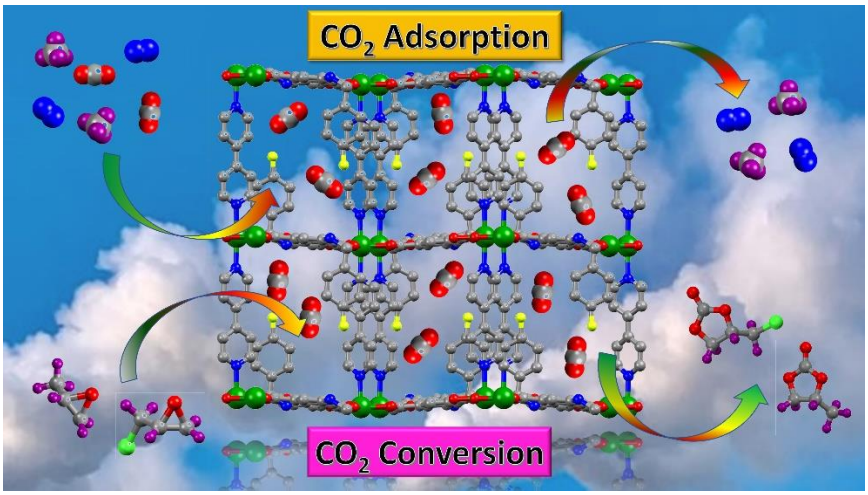

Figure 1: Functionalized 3D Cd(II) metal organic frameworks for effective and selective CO_2 adsorption and conversion.

Acknowledgements
This work was supported by the Fundação para a Ciência e Tecnologia (FCT) [2022.02069.PTDC, UIDB/00100/2020, UIDP/00100/2020 of Centro de Química Estrutural and LA/P/0056/2020 of Institute of Molecular Sciences projects] and by the Instituto Politécnico de Lisboa (IPL/IDI&CA2023/SMARTCAT_ISEL). A. Karmakar express his gratitude to Instituto Superior Técnico and FCT for Scientific Employment contract (Contrato No: IST-ID/107/2018) under Decree-Law no. 57/2016.

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KN6

Sustainable catalytic processes for CO_2 valorization

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Scientific topic: Homogeneous catalysis; Heterogeneous Catalysis; Porous materials for energy and environment

Carbon dioxide (CO_2) is one of main greenhouse gases, whose increasing emissions due to anthropogenic action constitute one of the most serious environmental problems the World faces, with consequent climatic, social and economic issues.[1] Therefore, besides the need to implement strict environmental policies and to change the society's mentality and lifestyle, modern chemistry plays a key role regarding the discovery of efficient strategies and technologies to mitigate CO_2 emissions, by capturing it and use it as a renewable "building block" in sustainable synthetic processes for preparation of value-added products (VAPs).[2]
Particularly, catalytic CO_2 addition reactions to epoxides deserve special attention, since these processes allow to obtain cyclic carbonates or polycarbonates, both of them with relevant applications, namely as green solvents and in plastic engineering, respectively.[3,4]
However, despite the remarkable progresses achieved over the last two decades regarding CO_2 capture and conversion, there is a lack of efficient and reusable catalysts and sustainable processes for the straightforward/sequential transformation of CO_2 into VAPs.
In this communication, we describe our recent works regarding the development of homogeneous and heterogeneous catalysts for CO_2 addition reactions to epoxides to selectively obtain cyclic carbonates and polycarbonates. We also present our recent achievements regarding the optimization and implementation of sustainable continuous-flow sequential processes involving CO_2 as renewable gas reagent.[5]

Acknowledgements
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KN7

C–N bonding formation mediated by transition metals: a useful tool to modify the porphyrin core

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Scientific topic: Other application(s)

The advancement of methods for incorporating nitrogen-based functionalities into organic frameworks is of utmost importance on synthetic chemistry research. Traditional methods for building carbon-nitrogen (C–N) bonds typically involve multiple steps, whereas metal-mediated C–N bond formation, like Ullmann and Buchwald-Hartwig cross-coupling amination approaches, has emerged as a breakthrough in efficiency and versatility. Over the past few decades, significant progress has been made in refining these approaches, establishing them as one of the most efficient synthetic routes for C–N bond building.[1,2]
These methodologies can be particularly attractive for modulating the physicochemical properties of porphyrins, including π-electron delocalization, thermal stability and susceptibility to electronic transfer, for specific applications like the development of photovoltaic devices.[3,4] In particular, 5,15-diarylporphyrins exhibit significant potential as hole-transporting materials (HTMs) for perovskite solar cells (PSCs) when properly functionalized. Consequently, numerous research groups have directed their efforts towards the synthesis and modification of these derivatives, aiming to introduce new and well-defined substitution patterns, such as electron-donor functionalities, that can make them alternatives to the benchmark Spiro-OMeTAD HTM.[4-6]
This communication will focus on the modification of the 5,15-diarylporphyrin core at *meso*-positions using nitrogen donor moieties through transition metal-catalyzed approaches to obtain *trans*-A_2B_2-type porphyrins containing *N*-donor heterocyclics or arylamines. The efficiency of resulting Zn(II)-based porphyrins as HTMs in PSC devices will be briefly discussed.[5]

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KN8

Carbon nanotubes derived from plastic solid waste: catalytic applications

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Scientific topic: Heterogeneous catalysis

Petroleum-derived plastics, ubiquitous across various industries, saw global production reach 367 million tonnes in 2021, with the EU accounting for *ca.* 30%. Polyolefins (polypropylene and polyethylene) dominate EU demand, particularly in single-use packaging, contributing to significant landfill buildup. Terrestrial plastic accumulation is projected to nearly triple by 2040, alongside a 2.6-fold increase in aquatic plastic pollution. A mix of traditional and innovative solutions is required to address this issue. Chemical recycling allows converting polymers into valuable monomers, supporting resource circularity. The high carbon content of plastics makes them valuable for production of materials like carbon nanotubes (CNTs), which are useful in catalytic processes such as catalytic wet peroxide oxidation (CWPO). CNTs, synthesized mainly via chemical vapor deposition (CVD), serve as active and stable catalysts in CWPO, although the impact of metallic impurities in CNTs remains underexplored. This keynote presentation will discuss the advances in the synthesis of CNTs using different metal substrates, polymer sources, CNT purification strategies, and environmental catalytic applications [1]. Through years of research, the group was capable to demonstrate the synthesis of CNTs using real low-density polyethylene solid waste (*cf.* Fig.1a,b), and their catalytic activity in CWPO for the removal of paracetamol, chosen as model micropollutant (Fig. 1c).

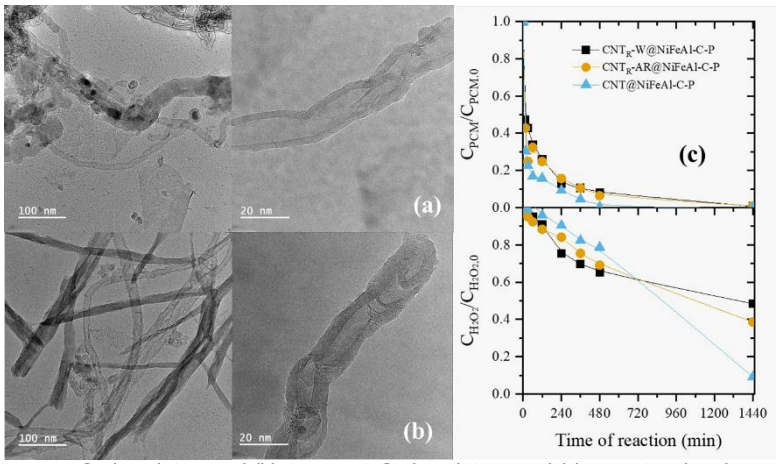

Fig. 1. TEM images of (a) CNT$_R$-W@NiFeAl-C-P and (b) CNT$_R$-AR@NiFeAl-C-P; and (c) CWPO using the samples.

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KN9

Functional porous materials for energy and biomedical applications

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Scientific topic: Preparation of new catalysts and/or porous materials

Nowadays, the research fields of energy and health are meeting global challenges in the quest to develop more sustainable, environmentally friendly, and well-being-oriented societies. These fields are crucial to achieve some of the seventeen goals outlined in the 2030 Agenda for Sustainable Development.[1] In relation to energy area, there is a critical need for clean and sustainable energy solutions based on greener processes, that can contribute for the reduction of harmful emissions and serve as alternatives to fossil fuels or efficient storage systems. On the other hand, in terms of health promotion, there is a demand for the development of more efficient drug formulations, therapies and diagnostic methods.
In this presentation, it will be shown several hybrid materials based on functionalized mesoporous silica nanoparticles (MSNs) and organic, metal, or pharmaceutical ionic systems that can have a wide range of applications. They can serve as desulfurization catalysts, components of dye-sensitized solar cells (DSSCs), electrolytes, photo(electrocatalysts) for hydrogen production, antimicrobial agents or for drug delivery.[2–8]

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ORAL COMMUNICATION ABSTRACTS

OC1

Depolymerization of plastic waste catalyzed by homogeneous and heterogeneous catalysts

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Scientific topic: Homogeneous catalysis

Modern society has become critically dependent on high-performance, low-cost plastics, which are essential for supporting our lifestyles. However, the increasing production and overuse of plastic packaging materials have led to severe environmental pollution problems.
Recycling plastic waste offers a two-way approach to sustainability, allowing both pollution reduction and the preservation of existing resources. To address this problem, significant efforts have been made to develop new strategies for recycling or extracting value from waste plastics.[1]
In continuation of our work,[2-7] in this communication will be presented the depolymerization of polyester and polycarbonate plastic waste into a variety of value-added compounds, relevant to the industry, catalyzed by homogeneous and heterogeneous earth-abundant catalysts (Figure 1).

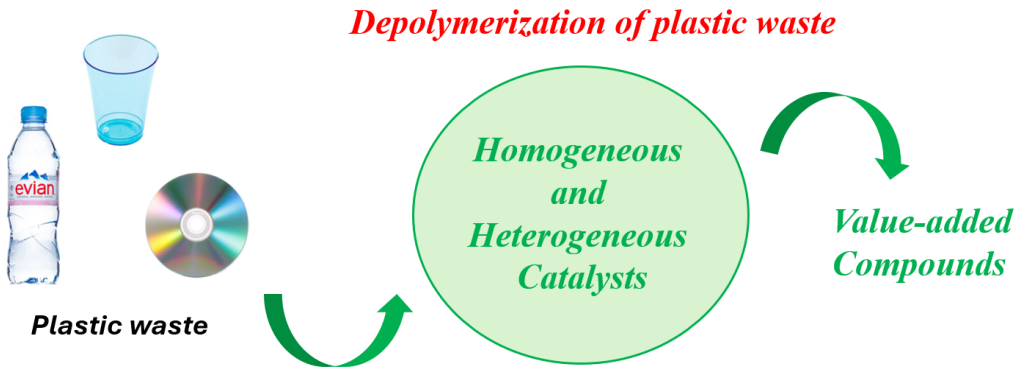

Figure 1: Catalytic conversion of plastic waste into value-added compounds.

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OC2

Transformation of biomass model compounds using Pt-Ni/Y catalyst prepared by mechanochemistry

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Scientific topic: Heterogeneous catalysis

Biomass is a renewable source with very high potential to produce biofuels that could replace, in a near future, fossil fuels. Although biomass can be transformed into bio-oil, the high oxygen content demands further transformation via hydrodeoxygenation (HDO) reaction to achieve adequate fuel properties[1]. Catalytic HDO occurs in the presence of bifunctional (metal + acid) catalysts, where the acid function can be provided by a zeolite and the metal sites can be introduced using several methods. Among them, mechanic mixture in ball mill (BM) has the advantage of being solvent-free, allowing to suppress solvent elimination and drying steps[2]. In this study, Ni/HY and bimetallic Pt-Ni/HY were prepared by mixing HY zeolite (Zeolyst, Si/Al=5.4) with $Pt(NH_3)_4Cl_2{\cdot}xH_2O$ and/or $Ni(NO_3)_2.\ 6H_2O$ in a planetary ball mil (Resch) using an agate vase with 5 spheres for 30 min and 200 rpm. The samples were calcined and reduced with H_2 at 450 ºC, being named as: *a*Pt, *b*Ni or *a*Pt-*b*Ni/HY, where *a* and *b* are the amounts of Pt and Ni (wt.%). The samples were characterized through powder XRD, N_2 adsorption at -196 ºC, TEM microscopy and laser diffraction particle sizing (LSD) measurements. The catalytic behavior in HDO reaction was studied using guaiacol as model molecule in a Parr 4843 batch reactor, with 200 mg of catalyst and 25 mL of 5 % vol. of guaiacol in *n*-heptane, at 250 ºC, 20 atm and 350 rpm. Samples were analyzed by gas chromatography equipped with FID detector and DB5-MS capillary column. X-ray patterns show that the milled samples kept the crystal order typical of Y zeolite, whereas LDS measurements (Fig. 1) clearly show a decrease in particle size upon milling. The catalytic results (Fig. 2) show that bimetallic catalysts, with low metal contents present an enhance catalytic conversion, when compared with monometallic Ni or even Pt, suggesting that the milling procedure promotes an intimate contact between the two metal species, with synergistic effects.

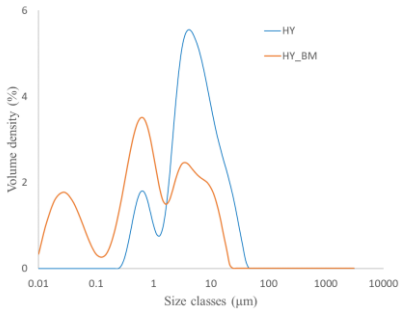

Figure 1: particle size distribution

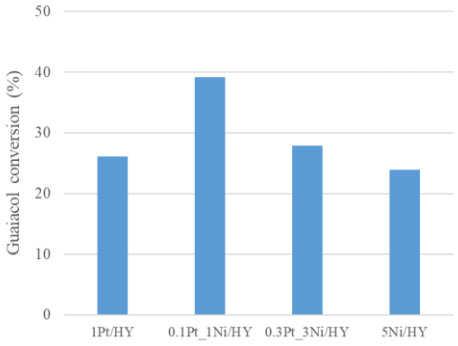

Figure 2: Guaiacol conversion after 60 min reaction

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OC3

Cork-derived activated carbon for environmentally friendly supercapacitors

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Scientific topic: Porous materials for energy and environment

The preparation of porous carbons, particularly from local, renewable, abundant, and cheap biomass, attracts a great deal of attention given the importance of these materials in many emerging applications, such as hydrogen storage, CO_2 capture, and energy storage in supercapacitors and batteries[1]. Cork is a biobased material of excellence, cheap, abundant in the South of Europe, and easy to obtain from wastes of the cork industry (Portugal is the world's largest producer). This work is part of the CORKCap project that aims to develop a new generation of eco-sustainable activated carbons (AC) derived from cork and the formation of composites with MnO_2 for asymmetric supercapacitor electrodes. An eco-friendly solvent-free route for converting cork waste into AC with a tailored porous structure is reported here. Combining chemical and physical activation and the presence of a nitrogen precursor to induce electrical conductivity of the AC[3], cork-derived AC electrodes were produced with considerable specific surface area (up to 1306 $m^2\ g^{-1}$ and a micropore volume of ca. 0.57 - 0.96 $cm^3\ g^{-1}$). The ratio between raw cork and the activating agents, physical or chemical activation temperatures, flow-rates, residence times, and heating rates used to generate adequate textural properties for enhanced electrochemical activity are presented. The cork-derived AC have been tested as electrodes in a symmetric two-electrode cell supercapacitor device and electrochemically characterized by cyclic voltammetry tests, galvanostatic charge-discharge measurements, and electrochemical impedance spectroscopy. Specific cell capacitances higher than 30 F g^{-1} were obtained using the prepared cork-derived AC; a commercial YP80 material characterised in the same device reached 33 F g^{-1}. Nevertheless, the cork-derived sample with the highest capacitance showed lower power density (~980 $W\ kg^{-1}$) compared to YP80 (~5000 $W\ kg^{-1}$), which may be due to the low conductivity (<0.06 S m^{-1}, measured by a four-point probe) observed for the prepared AC.

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OC4

From combustion residues to magnetic catalysts: innovative tool for water pollutant valorization

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Scientific topic: Heterogeneous catalysis

Coal fly ash (CFA) is an abundant coal combustion by-product with 750 Mt/y being produce worldwide.[1] However, approx. 75% of the CFA is landfilled.
Due to its good thermal stability and metallic oxides content (e.g., Fe_2O_3, SiO_2), bulk CFA has been pointed out as a material with high potential for heterogenous catalysis, while its Fe-rich magnetic fraction (CFA-Fe) is even more stable regarding catalytic physico-chemical properties.[2]
Currently, the extensive use of highly toxic and carcinogenic aromatic nitro compounds by various industries (e.g., dyes, pesticides), led to contamination of water bodies, which require treatment (adsorption/desorption, biological processes, and catalytic reduction). An advantage of the catalytic reduction of 4-nitrophenol (4-NPh) comparatively to other processes is the selective formation of 4-aminophenol, which is significantly less toxic than 4-NPh and has a high market value since it is used in the production of agrochemicals and pharmaceuticals (Fig. 1).
Good results were obtained using bulk CFA as catalysts or as catalysts support, e.g., for Pd NPs.[3] However, the potential of CFA-Fe on 4-NPh reduction was not assessed yet. Here, pristine CFA-Fe as received, pre-treated (water, NaOH and $NaBH_4$), and modified (composites with $CuFe_2O_4$) were tested as catalysts for 4-NPh valorization. Multi-technique characterizations (XRF, SEM-EDS, Raman, FTIR, XRD) confirmed the successful preparation of the materials. The as received CFA-Fe shows catalytic activity toward 4-NPh reduction and can be used up to 5 cycles, without efficiency losses (4-NPh conversion of 100%, 180 min). Compared to these, the samples pre-treated with NaOH and $NaBH_4$ showed enhanced catalytic performance (reaction time 5-60 min vs. 180 min). The (CFA-Fe)-based composites with $CuFe_2O_4$ showed excellent catalytic activity (total 4-NPh reduction in 3 min) comparable to noble metals (e.g., Au, Pd, Pt) containing catalysts.

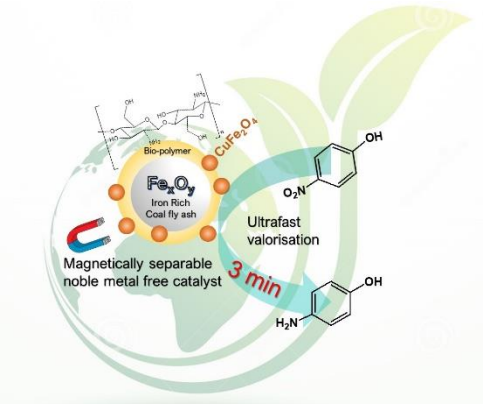

Figure 1. CFA-Fe based materials for catalytic reduction of 4-NPh.

Meanwhile, the recyclability (up to 5 cycles) of this (CFA-Fe)-$CuFe_2O_4$ composite is remarkable and it is easily recoverable *via* magnetic separation, which makes it a very promising material for being used at industrial-scale.

Fundings
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OC5

Ethylene photocatalytic oxidation for fruit ripening mitigation using TiO_2-based zeolite materials

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Scientific topic: Photocatalysis

Fruit ripening is caused by ethylene, a natural fruit hormone produced during the respiration process[1]. The common technologies used by industry to control the levels of ethylene are ventilation and controlled atmosphere chambers[2], but in both cases, traces of ethylene can still be faced. Photocatalytic oxidation of ethylene can be a cheap but efficient alternative. Due to its high efficiency and low cost, TiO_2 is commonly used for pollutant elimination. However, TiO_2 has one major limitation, that is its low ethylene adsorption[3]. To address this limitation, TiO_2 can be supported onto zeolites to increase TiO_2 dispersion and pollutant adsorption[4].

In this work, the TiO_2-ZSM-5 system was studied for the photooxidation of ethylene. TiO_2 (30 wt. %) was introduced in the zeolite via sol-gel method. A TiO_2 bulk was also prepared. Three temperatures for calcination were also studied (450, 550, and 650 ºC). The experiments were performed under a continuous gas flow system, where the photocatalyst was coated onto 4 glass tubes (20 mg catalyst) and further placed inside the tubular reactor. The gas composition was 300 ppm of ethylene, 21 vol. % of oxygen, and argon to complete 100 %. Two different lights were used, UVC (250 nm) and UV-visible (300-700 nm). XRD results showed that the composites present peaks from the zeolite and stabilized TiO_2 anatase phase (rutile phase not detected), with a sharpening of the anatase peaks (sintering), when increasing calcination temperature. Figure 1 shows the ethylene conversion (left) and the activity of the composites (right) compared with P-25. The results show that all the composites have a lower conversion than P-25. However, the composite calcined at 450 ºC has a conversion very close to P25 (96 % for P-25 and 91 % for 30 TiO_2-ZSM-5 450) that can be explained by the presence of very small anatase particles well dispersed, increasing the light absorption efficiency and the number of photoactive TiO_2 species. The composites TOF values showed a huge increase in TiO_2 activity, showing the beneficial effect of zeolite in dispersing TiO_2 and concentrating ethylene (increasing of the contact between TiO_2 species and ethylene).

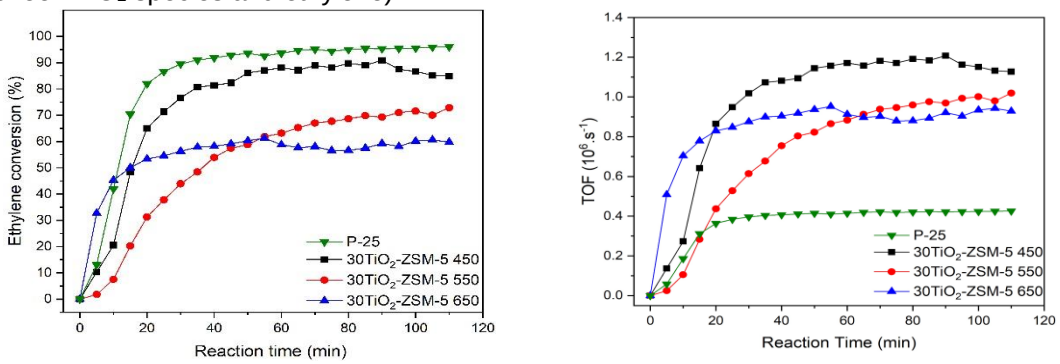

Figure 1: Ethylene photocatalytic oxidation conversion (left) and TOF values (right) for P-25 and composite 30TiO_2-ZSM-5 calcined at different temperatures (UVC illumination).

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OC 6

Crude glycerol: using acid zeolites to obtain fuel additives

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Scientific topic: Heterogeneous catalysis

Since the Industrial Revolution, fossil fuels have been the major source of energy.[1] However, biodiesel has become one of the most important and valuable alternative liquid fuels. For every 10 kg of biodiesel produced, about 1 kg of glycerol is generated as a byproduct. Thus, with the continuous increase in glycerol production, the current market struggles to absorb the excess supply.[2] A potential and promising application for glycerol derivatives lies in the automotive sector. Specifically, glycerol acetals, with solketal in particular, have been recognised as valuable fuel additives. Solketal is a 100% bio-based chemical derived from the acetalization of glycerol with acetone.[3-5] Zeolites, due to their excellent chemical and thermal stability, strong acid sites and industrial production, stand out as the most promising catalysts for acetalization reactions (Figure 1).

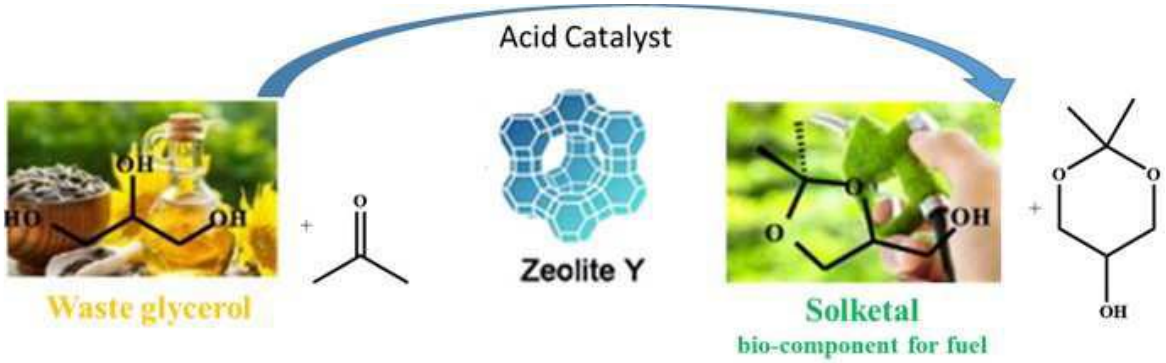

Figure 1 – Acetalization reaction of glycerol in the presence of acid zeolites**.**

The solvent-free synthesis of solketal from pure glycerol and acetone on a batch reactor, at 25 ºC, using HZSM-5 and HY zeolites with different ratios of Si/Al has been studied. The best performance concerning glycerol conversion and selectivity to solketal was registered with HY60 after 10 min of reaction, 82% of conversion, and 98% selectivity for solketal. Also, the reusability of HY30 and HY60 was evaluated through 13 catalytic cycles. HY60 zeolite remained active for 13 cycles.
The stability of the catalysts was studied between cycles using powder-XRD, and after the 6th and 13th cycle by 1H, 29Si and 27Al NMR. Certain factors like the presence of water in the catalysts were also studied, to better understand the reaction dynamics and mechanism. Incorporating this knowledge, new experiments were conducted with HY60 catalyst, this time utilizing crude glycerol supplied by PRIO-Aveiro, Portugal. The glycerol, collected at various stages of its purification process, yielded very promising results.

Acknowledgements
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OC7

Mechanochemistry and catalysis, a powerful alliance for the development of sustainable processes

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Scientific topic: (Preparation of new catalysts and/or porous materials

Mechanochemistry is the study of physicochemical transformations driven by mechanical energy. Although mechanochemical reactions have been known since ancient times, the capability to promote the reaction under solvent-free conditions, whose benefits go beyond waste prevention, have attracted the attention of synthetic chemists searching for sustainable synthetic processes.[1] Catalysis is central in Green Chemistry, driving chemical transformations by accelerating reactions, reducing energy requirements, and minimizing waste, thus enabling a decrease in environmental impact and resource consumption, and facilitating chemical transformations with higher efficiency and selectivity. Mechanochemistry has been used as a tool to develop sustainable processes for the synthesis of pro-ligands, however, the alliance of mechanochemistry with catalysis goes beyond the synthesis of catalysts under mechanochemical conditions. In this presentation some examples of our research on the mechanochemically assisted synthesis of *N*-heterocyclic pro-ligands, catalysts and catalyzed reactions will be presented, as well as the improvement in sustainability evaluated through the analysis of green chemistry metrics, Figure 1.[2]

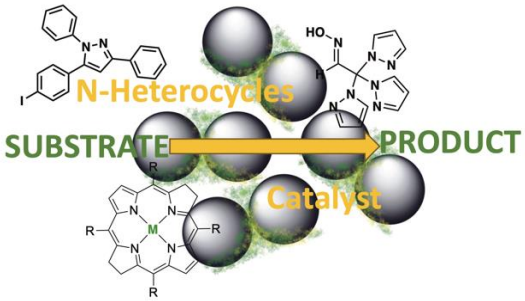

Figure 1: From the ligand to the catalyst and the catalyzed reaction under mechanochemical action.

Acknowledgements
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OC8

Biodiesel additives synthesis using metal(IV) phosphates catalysts: Esterification of levulinic acid

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Scientific topic: Heterogeneous catalysis

Introduction. Fossil fuels still dominate the energy market. But, the depletion of fossil resources increased the search for renewable alternatives. Among several biomass-based chemicals, levulinic acid (LA) and levulinic esters (LEs) are important platform compounds with wide application, such as fuel additives. The esterification of LA and biomass derivatives can be easily performed if catalysed by different solid acids. The acidic nature of metal(IV) phosphates enclose all the characteristics to act as efficient solid catalysts[1,2].

Experimental/methodology. Our work started with the synthesis and characterization of the α- and γ-zirconium phosphates (α- and γ-ZrP). Then, the catalytic performance of these catalysts was evaluated in the esterification reactions of LA with ethanol (EtOH) or methanol (MeOH) using the conventional reflux method (CV). Different LA:EtOH or LA:MeOH molar ratios and catalyst:LA mass ratios were studied at 78 °C and 65 °C during 6 hours. Four products, 5-ethoxy-5-methyldihydrofuran-2-one (ethoxy-PL), ethyl levulinate (EL), 5-methoxy-5-methyldihydrofuran-2-one (methoxy-PL) and methyl levulinate (ML) were formed.

Considering the LA conversion, the best results with the α-ZrP were achieved with a α-ZrP:LA mass ratio of 30% and a LA:MeOH molar ratio of 1:10 (Figure 1). With the γ-ZrP, the best results were achieved with a γ-ZrP:LA mass ratio of 30% and a LA:EtOH molar ratio of 1:20 (Figure 1). Blank reactions were also performed for these conditions.

Considering the former best parameters, the esterification reactions of LA were performed by the microwave assisted method (MW) at 80 °C and 100 °C during 2 hours (Figure 1). Good results were obtained with the α-ZrP at 100 °C with methanol and the γ-ZrP at 80 °C with ethanol. Blank reactions were also performed in the same conditions. Given the good results obtained after 2 hours by the MW, the reactions reffered above were choosen to be monitored each half an hour (Figure 2).

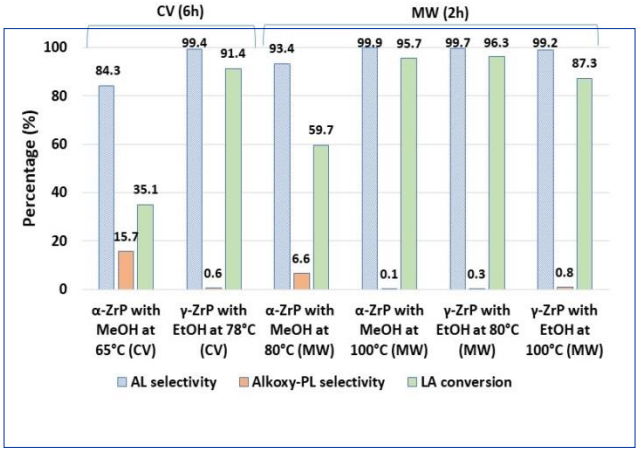

Figure 1: CV versus MW reactions

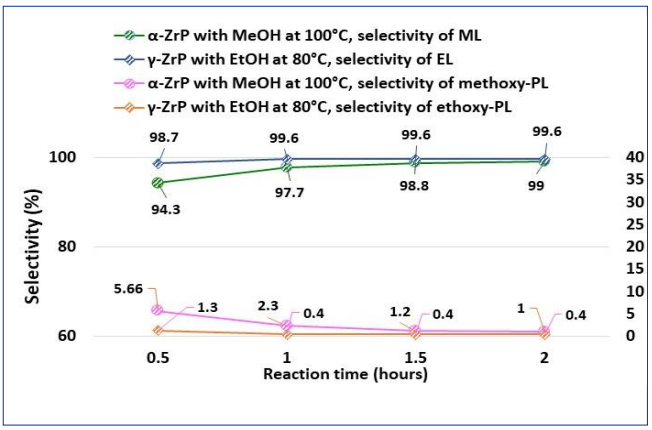

Figure 2: monitoring reactions

Results and discussion. The best LA conversions and alkyl levulinates (AL) selectivities were obtained by the MW after 2 hours of reaction either for the α-ZrP or γ-ZrP (Figure 1). These results are really good considering that the reaction time was substantially decreased from 6 to 2 hours, with both catalysts, which implies a considerable decrease in energy and water consumption. The results shown in Figure 2 are even more enlightening since it was verified that the monitored reactions start to give very good results even after 1 hour of reaction making our catalysts very promising in a near future.

The formation of the alkoxy-PL intermediates could compromise the formation of the AL in good yields. However, this step has been successfully overcome due to the perfect combination of several parameters (catalysts, molar ratio LA: EtOH, mass ratio catalyst:LA, temperature, time of reaction and method used).

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OC9

Sustainable fuel desulfurization using advanced porous catalytic membranes

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Scientific topic: Porous materials for energy and environment

A recent analysis conducted by the U.S. Energy Information Administration anticipates that fossil fuels will maintain their predominant role in global energy production, accounting for approximately 70% by the year 2050.[1] The burning of fossil fuels leads to harmful environmental emissions, such as sulfur oxides, which contribute to climate change, particularly acid rain. While hydrodesulfurization (HDS) methods have traditionally been employed to remove sulfur from road fuels, finding alternative desulfurization techniques becomes imperative for heavy fuel oils, as traditional methods often prove inefficient due to their unique composition. Exploring these alternatives is crucial for petroleum refineries to mitigate waste production by valorizing the heavier distillation residues. Oxidative Desulfurization (ODS) has emerged as a remarkably efficient method for sulfur removal from fuels, functioning at significantly reduced temperatures and pressures in comparison to HDS. Sustaining ODS's efficiency entails exploring novel catalysts such as polyoxometalates (POM), which have shown remarkable effectiveness in driving these reactions.[2] Nevertheless, the powdered form of these catalysts has been a significant hurdle, impacting their ease of handling and recyclability. To overcome this limitation, innovative membranes that embed POMs within porous polymeric membranes were designed. This work focuses on the rapid and straightforward fabrication of these catalytic membranes and their application in successful desulfurization of model fuels. Employing these groundbreaking membranes not only improved the stability of catalysts but also extended their operational lifespan by reducing mass loss. Notably, the catalytic membrane strategy markedly boosts performance compared to traditional bulk catalysts (Figure 1), highlighting the substantial potential of catalytic membranes. This study establishes a foundation for advancing ODS at an industrial level and offers promising prospects for more eco-friendly and efficient fuel desulfurization processes.

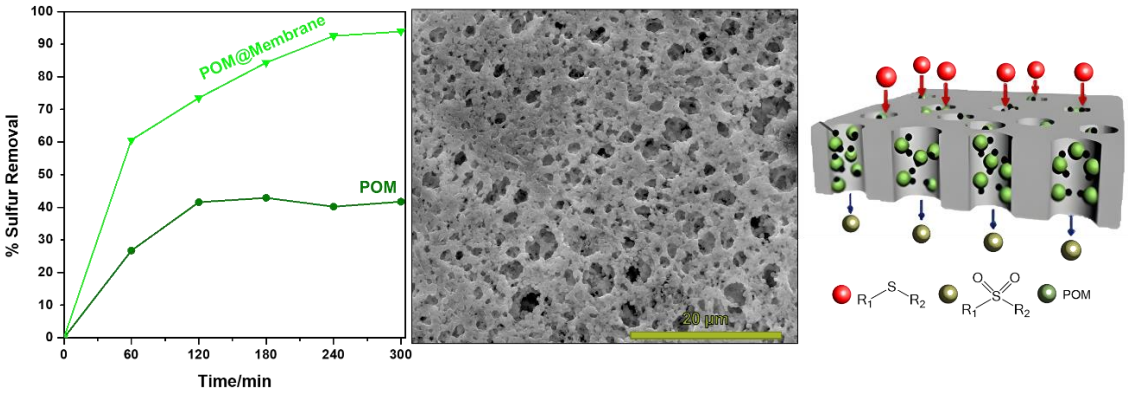

Figure 1. Comparison of catalytic profiles: POM vs. POM@Membrane (left). SEM image of a porous catalytic membrane (center). Illustration of the reaction occurring within a porous catalytic membrane (right).

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OC10

Chlorophyll as a natural photocatalyst to obtain antimicrobial compounds from rosin oxidation

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Scientific topic: Photocatalysis

Pathogenic microorganisms' resistance to antibiotics poses a serious threat to both human and animal health. The search for novel bioactive agents, such as natural compounds and their derivatives, has been a major focus of research in recent years.

Gum rosin, also known as colophony, is a natural, abundant, cheap, and non-toxic raw material that is obtained as a solid residue after distillation of pine resin. It is composed of 90-95% of diterpenic resin acids, which are known to present several biological activities, namely anti-inflammatory, antiulcer, cardiovascular protection, and antimicrobial.[1] Some authors have described that the presence of hydroxyl or carbonyl functions in the resin acids molecules are features for the expression of antimicrobial activity.[2] Despite the great importance of oxidized resin acids, their natural occurrence is limited. Therefore, the oxyfunctionalization of resin acids present in rosin can conduct to significant amounts of these compounds and to better biocidal features.

In this work, it will be discussed the photocatalytic oxidation of rosin isolated from *Pinus elliottii* using chlorophylls as natural photocatalysts. Studies concerning the extraction of chlorophyll derivatives from natural sources and the conditions used to perform the photocatalytic oxidations will be presented. A special attention will be given to the oxidized products obtained in the presence of crude chlorophyll extract or of purified chlorophyll. A brief reference to the *in vitro* antimicrobial activity of the oxidized rosin towards *Staphylococcus aureus*, *Clostridium perfringens*, *Penicillium* sp., and *Escherichia coli* will also be presented.

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OC11

Rapid formation of vinylene-linked phenanthroline covalent organic frameworks for photocatalysis

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Scientific topic: Preparation of new catalysts and/or porous materials

Covalent organic frameworks (COFs) are an emerging class of crystalline porous materials that have shown to be promising platforms for catalysis due to their tunable and well-defined structures, high surface areas, and low density.[1] Particularly, vinylene-linked COFs are very interesting for photocatalysis owing to their efficient π-electron delocalization over the robust C=C bonds, offering high chemical stability and unique optoelectronic properties, like narrow band gap structures and rapid charge carrier mobility.[2] However, most reported syntheses of these COFs typically involve solvothermal methods that require controlled atmosphere and pressure conditions in a sealed Pyrex tube, which can be time-consuming and hinder their scalable production. Recently, solid-state synthesis using benzoic anhydride as the catalyst has gathered attention for being an efficient and more sustainable approach for COF synthesis. However, this approach still suffers from long reaction times ranging from 3 to 5 days.[3]
In the present study, we report the rapid and solvent-free synthesis of three novel vinylene-linked COFs driven by the pre-organization of 4,7-phenanthroline (Phen) monomers via efficient intermolecular forces, boosting the formation of crystalline products in merely 30 min (Figure 1). The successful formation of the materials was validated through various characterization techniques in terms of their crystallinity, textural properties, chemical connectivity, and optical properties. The prepared COFs exhibited broad visible light absorption, narrow optical band gaps, and demonstrated photocatalytic activity in dye degradation, indicating their potential for visible-light-driven applications.

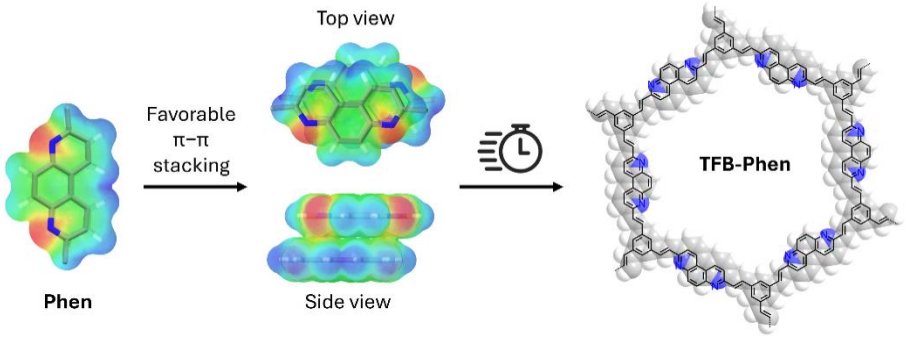

Figure 1: Schematic illustration of the pre-organization of Phen monomers.

Acknowledgements
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OC12

Green aromatic epoxidation with an iron porphyrin catalyst for functionalization of renewable xylene, quinoline, and acridine

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Scientific topic: Homogeneous catalysis

An important step in implementing a circular economy and reducing the chemical industry's reliance on petrochemicals as raw materials is the valorization of compounds derived from renewable sources. Additionally, the use of biomimetic catalysts based on non-noble metals allows mild and eco sustainable conditions for efficient and selective reactions. [1] In this work, the biomimetic one-pot oxidation of typically inert aromatic compounds obtained from renewable sources, namely *o*-xylene, quinoline and acridine, was performed using a highly electron withdrawing iron porphyrin catalyst (Figure 1).

The functionalized aromatic compounds were obtained with high yields, in the absence of additives, under room temperature and with ethanol and hydrogen peroxide as green solvent and oxidant, respectively. The results indicate the occurrence of aromatic ring epoxidation. The epoxides were isolated or evolved through rearrangement, ring opening by nucleophiles, and oxidation. o-Xylene was oxidized to 4-hydroxy-3,4-dimethylcyclohexa-2,5-dienone, an attractive building block for synthesis, and 3,4-dimethylphenol as an intermediate, with TON of 237. Quinoline was directly functionalized to 4-quinolone or 3-substituted-4-quinolones, which have high potential for biological activity, and corresponding hydroxy-tautomers, with TON of 61. Acridine was oxidized to mono- and di-oxides in the peripheral ring: 1:2-epoxy-1,2-dihydroacridine and anti-1:2,3:4-diepoxy-1,2,3,4-tetrahydroacridine, with TON of 285. [2]

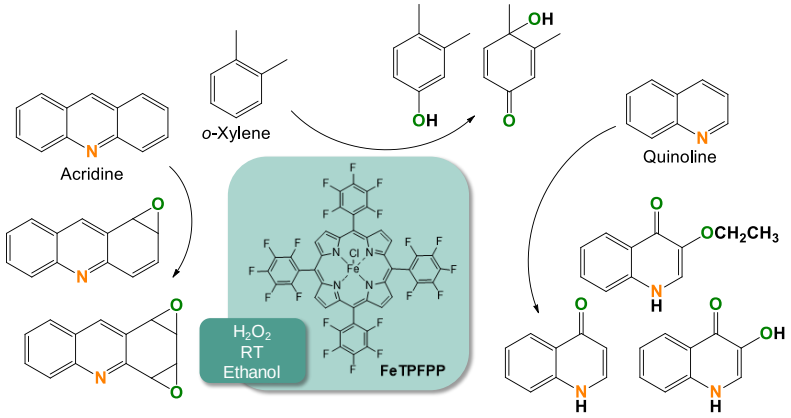

Figure 1: Biomimetic oxidation of renewable aromatics.

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Acknowledgements
We thank FCT/MCTES support (LA/P/0008/2020 DOI 10.54499/LA/P/0008/2020, UIDP/50006/2020 DOI 10.54499/UIDP/50006/2020 and UIDB/50006/2020 DOI 10.54499/UIDB/50006/2020, through national funds). S.L.H. Rebelo thanks FCT for funding through program DL 57/2016—Ref. REQUIMTE/EEC2018/30 and G.A. Corrêa thanks FCT for her PhD grant (UI/BD/154487/2022).

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OC13

Sustainable approaches for CO_2 catalytic conversion into fuels and valuable products

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Scientific topic: Nanocatalysis

The emergence of carbon dioxide methanation as a promising strategy for mitigating greenhouse gas emissions and promoting carbon utilization (CCU) is a significant development in the context of global climate challenges. This process not only helps reduce CO2 emissions but also facilitates the generation of renewable energy by converting carbon dioxide into methane, thereby offering a pathway towards carbon neutrality [1].
Through CO_2 hydrogenation, a wide range of chemicals can be obtained, including formic acid, formate, methane, lower olefins, higher hydrocarbons, methanol, higher alcohols, and others, many of which can serve as fuels. However, a major obstacle in CO conversion lies in its stability as a molecule, which necessitates a significant amount of energy for activation. By employing a biphasic system containing excess CO in the gas phase and imidazolium ionic liquid (IL) in the stationary phase, CO methanation can be achieved at relatively mild temperatures. The unique properties of ILs promote the formation and stabilization of highly active ruthenium nanoparticles capable of catalyzing the reaction, resulting in an 84% yield at 150ºC after optimization [2, 3].
Recent studies have explored various approaches to enhance the efficiency and sustainability of this reaction, including the use of deep eutectic solvents as alternative media or covalent organic frameworks (COFs) as porous catalytic supports. Some of these catalytic strategies are being developed for continuous processes in collaboration with industrial partners. Additionally, other CO_2 catalytic approaches are being investigated, such as the electroreduction of CO_2 to syngas in aqueous IL media [4] and cyclic carbonate formation in homogeneous or heterogeneous processes in the presence of IL media [5].
These advancements represent significant steps towards developing more efficient and sustainable methods for carbon dioxide utilization, which could play a crucial role in addressing climate change and promoting the transition towards a low-carbon economy (Figure 1).

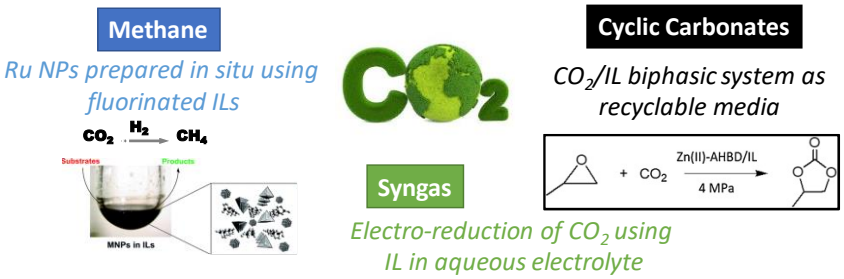

Figure 1: CO_2 catalytic conversion into fuels and valuable products

Acknowledgements
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OC14

Synthesis of functional polymers for selective adsorption of bioactive compounds from olive leaf extracts

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Scientific topic: Porous materials for energy and environment

Olive leaves are a significant part of the generated residues in the olive market, these leaves possess a plethora of bioactive compounds that worth their valorization for application in the food, feed, chemical, nutraceutical, cosmetic and pharmaceutical sectors[1]. Irrespective to the method employed to get the bioactive compounds in olive leaf (hydroalcoholic, organic solvents, $SCCO_2$, etc.), a mixture of diverse compounds is obtained at the end. Considering this issue, the implementation of tailored sorbents in sorption/desorption processes provides improvements in selectivity and loading capacity towards selected compounds. Herein, the synthesis of a molecularly imprinted polymer (MIP), using quercetin as a template, followed by its integration in the sorption/desorption process of a real olive live extract was demonstrated. The inverse suspension polymerization was the adopted polymerization mechanism. The used methodology allowed to scale up the MIP production to the gram-scale to work with preparative columns, and control of the particle size to prevent potential back-pressure issues when running continuous processes[2]. The results point to the usability of the synthesized sorbent to fractionate the initial extract, at a moderate temperature (45ºC) using hydroalcoholic solvents (ethanol-water mixtures).
This research group has already demonstrated the functionalization and implementation of these materials for the purification/concentration of bioactive compounds in the framework of circular bioeconomy, namely, to get high-added-value compounds from olive leaf or other kinds of agricultural residues[2,3].

Acknowledgements
We acknowledge the support through the OLEAF4VALUE project. This project has received funding from the Bio-Based Industries Joint Undertaking under the European Union's Horizon 2020 research and innovation programme under grant agreement nº 101023256. Ayssata Almeida acknowledges FCT for the PhD scholarship PRT/BD/154653/2022. Catarina Gomes acknowledges FCT for the PhD scholarship 2020.06057.BD. We also thank to NATAC for providing the olive leaf extracts and the aid with the identification by LC-MS of compounds there contained. Rolando Dias is grateful to the Foundation for Science and Technology (FCT, Portugal) for financial support through national funds FCT/MCTES (PIDDAC) to CIMO (UIDB/00690/2020 and UIDP/00690/2020) and SusTEC (LA/P/0007/2020). Mário Rui Costa acknowledges the support by LA/P/0045/2020 (ALiCE), UIDB/50020/2020 and UIDP/50020/2020 (LSRE-LCM), funded by national funds through FCT/MCTES (PIDDAC).

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OC15

Advanced smart textiles: Electrochromic supercapacitors boosted by glucose-derived carbon and PEDOT:PSS

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Scientific topic: Porous materials for energy and environment

The core shift of the energy is the transition from fossil fuel systems to renewable alternatives, while advancing clean energy technologies to ensure a sustainable future. Supercapacitors (SCs) emerge as a promising solution for energy storage, featuring extended cycle life and fast charging. However, the development of multifunctional SCs with sensing properties for real-time monitoring of energy consumption is still a challenge. To address this issue, bifunctional devices with energy storage capabilities and the ability to reversibly change color under an applied potential, namely electrochromic SCs (ECSCs) are being developed.[1]

In this study, we developed symmetric and asymmetric ECSC devices with planar structure using cotton textiles coated with electrically-conductive polymer poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) and N-doped glucose-derived carbon/multiwalled carbon nanotubes (CNTs) as electrode materials and a gel polymer electrolyte. The N-doped glucose-derived carbon/CNT hybrid material was prepared through hydrothermal carbonization of glucose in the presence of 2 wt% of CNTs. It exhibited high specific surface area (1381 $m^2\ g^{-1}$), large volume of micropores (0.56 $cm^3\ g^{-1}$) and was composed of spherical particles (274±52 nm) and well-dispersed CNTs.

All the fabricated devices demonstrated successful energy storage properties. The asymmetric ECSC demonstrated an energy density of 5.5 µWh cm^{-2} at a power density of 1039.9 µW cm^{-2}, which were 81% and 65% higher, respectively, than the values obtained for the symmetric ECSC device based on PEDOT:PSS. In terms of electrochromic properties, the symmetric device based on PEDOT:PSS and the asymmetric device (Fig. 1) exhibited the most notable color change for potential values higher than |±1.2| V.

This research opens new pathways for the development of textile-based devices with supercapacitive and electrochromic properties for wearable electronics.

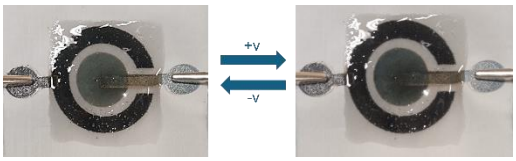

Fig. 1: Asymmetric ECSC textile based on glucose-derived carbon and PEDOT:PSS electrode materials.

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1357 04968/2020). GPQ thanks FCT for the PhD scholarship (UI/BD/151274/2021). CRP thanks FCT for funding through Individual Call to Scientific Employment Stimulus, ref.2021.04120.CEECIND/CP1662/CT0008 (DOI: 10.54499/2021.04120.CEECIND/CP1662/CT0008).

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OC16

Polyoxotungstates@MIL-100(Fe) to achieve sustainable oxidative desulfurization and denitrogenation of fuels

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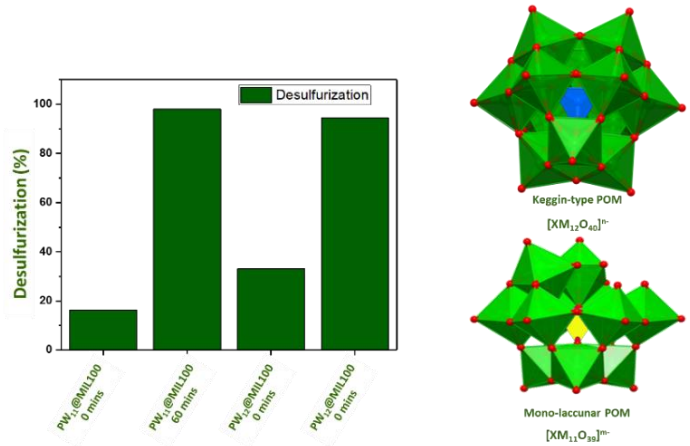
Scientific topic: Heterogeneous Catalysis

The need to mitigate environmental pollution drives the continuous quest for advanced desulfurization and denitrogenation methods in the refining industry. The presence of sulfur (S) and nitrogen (N) compounds in fossil fuels not only contributes to atmospheric pollution but also reduces the performance of catalysts and downstream equipment.[1] Oxidative catalysis presents a promising way for addressing these challenges, offering efficient and environmentally-friend pathways for sulfur and nitrogen removal.[2] In this study, we investigate the heterogeneous catalytic performance of two different types of Polyoxometalates (POMs) – Keggin PW_{12} and lacunar PW_{11} structures, supported in MIL-100(Fe) metal-organic framework (MOF), for simultaneous oxidative desulfurization and denitrogenation of a model fuel. Both PW_{11}@MIL-100(Fe) and PW_{12}@MIL-100(Fe) heterogeneous catalysts demonstrated rapid and complete desulfurization within 60 minutes of reaction, using only 100 µL of extraction solvent and H_2O_2 as oxidant. Remarkably, PW_{11}@MIL-100(Fe) exhibited highly catalytic efficiency over 5 cycles. In comparison, PW_{12}@MIL-100(Fe) displayed diminished activity after the third cycle. This work presents remarkable results, showing that the application of oxidative catalysis is a promising sustainable direction to achieve S and N removal from fuels, offering insights for the development of efficient and reusable heterogeneous catalysts in the petroleum industry.



Scheme 1 – Scheme of catalytic efficiency comparing two different Keggin-type Polyoxometalates – mono-lacunar and plenary, PW_{11}@MIL100-(Fe) and PW_{12}@MIL100-(Fe), respectively.

Acknowledgements
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Funds
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OC17

The participant cancelled his presence

OC18

Synthesis of 2-methylresorcinol-based cavitands by means of homogeneous catalytic reactions

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Scientific topic: Homogeneous Catalysis

Bowl-shaped cyclotetrameric molecular containers are in the focus of our recent investigations. In addition to high-yielding synthetic reactions, transition metal catalysed homogeneous catalytic ones are combined to synthesize deepened cavitands. To achieve this goal, upper rim functionalization of cavitands bearing iodoarene, vinylarene anf ethinylarene moieties were used as substrates in transition metal-catalysed reactions. In addition, an approach *to investigate unprecedented supramolecular catalytic synergies* has been in the focus of our research as well. Similar reactions have been sparsely employed to cavitands as convenient tools for molecular enlargement.[1] Based on our previous studies on palladium-catalysed aminocarbonylation and cross-coupling reactions on a of 2-methylresorcinol-based cavitand scaffold,[1f] further unexpectedly highly chemoselective reactions toward tetrafunctionalized derivatives will be presented.
Highly selective palladium-catalysed aminocarbonylations of simple and multilevel cavitands possessing 4-iodophenyl moieties on the upper were carried out. The amine nucleophiles range from simple primary amines (for example *tert*-butylamine) via amino acid esters to aminosteroids and aminosugars. High 'tetra-selectivity' was obtained in two aspects: a) tetracarboxamides and tetrakis(2-ketocarboxamides), formed via mono and double carbon monoxide insertion, respectively, were obtained exclusively, b) carboxamides/2-ketocarboxamides possessing the same *N*-substituent were formed even in those cases when two different amines as nucleophiles were used.[2]
Two types of cavitands possessing 4-vinylphenyl substituents (i.e., styrene moieties) were used as substrates in platinum- and rhodium-catalyzed hydroformylation reactions. Surprisingly, the reactions proceeded with high 'tetra-selectivities', that is, all four vinyl groups were either hydrogenated or transformed to the branched or linear aldehydes via hydroformylation. Based on these exceptionally high chemo- and regioselectivities, a cooperation between all the four catalytic reaction centers was supposed.[3]
Azide-alkyne (3+2) cycloaddition reaction ('click'-reaction) has been used routinly for the enlargement of the cavitand backbone.

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OC19

Porous MOF-based materials with high potential to sustainable catalytic processes

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Scientific topic: Preparation of new catalysts and/or porous materials

Metal–organic frameworks (MOFs), also known as crystalline porous coordination polymers, have been proven to be excellent contenders for bridging the gap between zeolites and mesoporous silica. MOFs are formed by metal ions/clusters and organic linkers and have captured widespread interest, achieving an explosive development over the past two decades. The crystalline nature, structural diversity, and tuneability, as well as ultrahigh surface area make MOFs find their potential applications in diverse areas, such as gas sorption and separation, chemical sensing, proton conductivity, biomedicine, and catalysis. However, in numerous MOFs the structural stability and performance limits their practical applications, relatively to other porous materials. Consequently, distinct strategies have been used to prepare MOF based materials and overcome these disadvantages.[1, 2]

The modification and derivation of MOFs, and their utilization as platform, template or subtract opens an avenue to the preparation of diversified porous materials with unique advantages in comparison to traditional pristine materials. Following our interest in the development and application of functional MOFs towards sustainable catalytic processes (both heterogeneous catalysis and electrocatalysis) an overview of MOF-based materials recently prepared and investigated in our research group is reported.

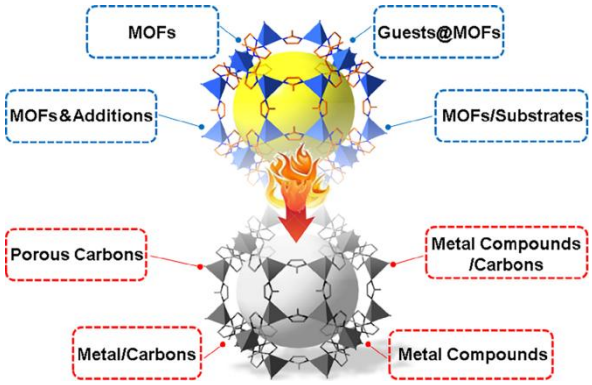

Figure 1. Illustration of the preparation of distinct porous materials from MOFs and MOF-based composites as templates/precursors. [2]

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OC20

Nanostructured binuclear catalysts and nanozymes by ionic self-assembly of first-row transition metalloporphyrins

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Scientific topic: Preparation of new catalysts and/or porous materials

Binuclear materials have been prepared in a simple and eco-sustainable way by ionic self-assembly of oppositely charged metalloporphyrins. The assembly process is driven by electrostatic interactions, hydrogen bonds and/or π-π stackings, which afford nanostructured materials with high specific surface areas.[1]
Cooperative processes might occur between the positive and negative tectons and lead to emergent or improved catalytic properties.[1,2] Moreover, porphyrins are chromophores with strong visible light absorption, thus enhanced photo-physical properties and donor-acceptor mechanisms can be attained.
In this work, binary porphyrin structures (BIPOS), composed by porphyrins carrying metal ion centers of the first-row transition series [Mn(III); Fe(III), Co(III), Ni(II) or Cu(II)], have been prepared and characterized by scanning electron microscopy, UV-visible spectroscopy, and electrochemical studies. Their catalytic performance has been evaluated in the activation of small molecules, namely in the H_2O_2 activation for novel nanozymes development with catalase- and peroxidase-like activity, as well as, in the $NaBH_4$ activation for catalytic hydrogenation of nitrobenzene in the presence and absence of visible light (Figure 1).[1,2]

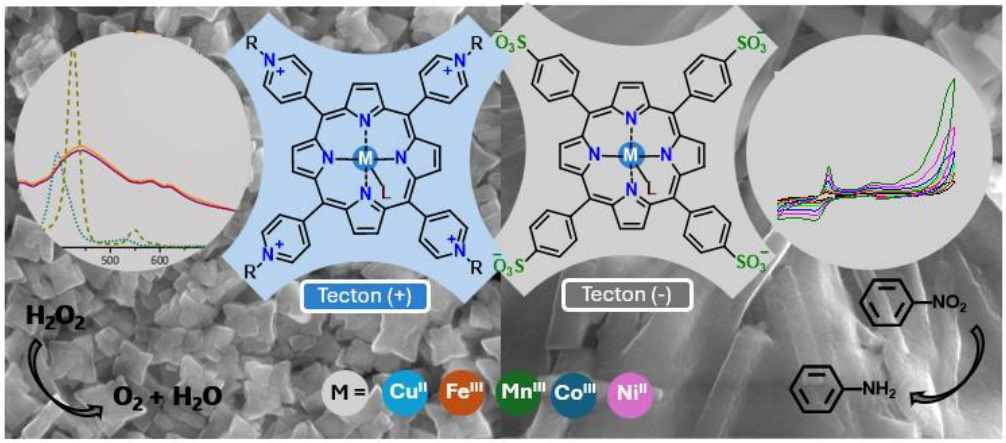

Figure 1: Binary porphyrin structures used in electrochemical and (foto)catalytic studies.

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OC21

CO oxidation on single-atom catalysts based on the molybdenum carbide (Mo_2CO_2) MXene

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Scientific topic: Heterogeneous catalysis

MXenes are two-dimensional transition metal carbides and nitrides.[1] Herein, we investigate, through density functional theory (DFT) calculations, the mechanism of CO oxidation to CO_2 on single-atom catalysts consisting of an atom of Fe, Ti or Zn deposited on the surface of the Mo_2CO_2 MXene.[2]
In the case of Fe@Mo_2CO_2, a mechanism resembling that of Termolecular Langmuir-Hinshelwood (TLH) is thermodynamically and kinetically favoured, displaying very exothermic CO_2 formation, low activation energies, and easy CO_2 desorption. On Ti@Mo_2CO_2, the dissociation of CO_2 is almost barrierless and much more likely to occur than CO_2 desorption, barring the usage of this surface as a catalyst for CO oxidation. Finally, on Zn@Mo_2CO_2, a hybrid Langmuir-Hinshelwood/Eley-Rideal (LH/ER) mechanism is thermodynamically and kinetically feasible. Here, after the first CO_2 forms, with an energy barrier of only 0.62 eV, the second CO_2 is formed spontaneously, and the Zn-CO_2 interactions are weak enough to allow desorption.
The calculated thermodynamic quantities and reaction rates at T = 300 K indicate that Fe@Mo_2CO_2 should be quite active towards CO oxidation, followed by Zn@Mo_2CO_2, while the Ti-based model is inactive. Our results add to the evidence that establishes single transition metal atoms adsorbed on MXene surfaces as cheap and easily obtainable catalysts that offer the best of both bare and functionalized MXenes.[3]

Acknowledgements
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OC22

Catalytic system for conversion of sugarcane molasses waste to 5-hydroxymethylfurfural

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Scientific topic: Heterogenous catalysis

Catalytic methods to transform industrial biomass waste into platform chemicals and materials are urgently needed to address the energy crisis and environmental issues linked with the extensive reliance on fossil fuels. In this sense, sugarcane molasses (SCM), a waste product from the sugar industry, can be transformed into a versatile biorefinery intermediate called 5-hydroxymethylfurfural (HMF) using multifunctional catalysts. The complex reaction pathway involves i) the hydrolysis of sucrose into glucose and fructose (catalyzed by Brønsted acid (BA) sites), ii) the isomerization of glucose into fructose (catalyzed by Lewis acid (LA) sites), and iii) fructose dehydration to HMF (catalyzed by BA sites) [1]. Several side reactions may also occur, including the acid-catalyzed HMF rehydration to organic acids and condensation or cross-polymerization of HMF with hexoses, forming soluble polymers and insoluble humin. The catalytic valorization of SCM can also be affected by the presence of non-sugar impurities in the feedstock, including colorants (i.e., melanoidins) and metal salts, which can hinder the catalytic reaction.

The present work was focused on maximizing the HMF yield obtained from SCM by optimization of the catalytic system and purification of the feedstock. A solid acid catalyst containing BA sites was prepared by hydrothermal carbonization in the presence of H_2SO_4 and abbreviated Cstarch_SO_3H. The catalytic performance of Cstarch_SO_3H was compared to that of HUKUST-1, a metal-organic framework containing mostly LA sites with some weak BA sites. The catalysts were tested in the conversion of SCM to HMF using a microwave reactor at 180 °C. Different pretreatments of SCM were considered to boost the HMF yields obtained, including purification with acids, centrifuging, and adsorption on activated carbon (AC).

The results obtained using as-received SCM demonstrated that HKUST-1 was the most promising catalyst, achieving a maximum HMF yield of 22% with a selectivity of 34% in a 30-minute reaction. In comparison, a maximum HMF yield of only 12% with a selectivity of 15% was obtained by Cstarch_SO_3H in a 20-minute reaction. It was found that centrifugation followed by adsorption on AC was the most effective purification method of SCM, which removed all colorants, organic compounds, and most metal ions. The catalytic tests using purified SCM showed an increase in HMF yield to 29% in the presence of HKUST-1 under the same reaction conditions. Finally, the highest HMF yield of 31% and an unpreceded selectivity to HMF of 52% were obtained by combining HUKUST-1 and Cstarch_SO_3H catalysts. The improved catalytic performance was attributed to synergistic effects between multiple acid sites with different types and strengths. Nevertheless, the recyclability tests identified low stability of HUKUST-1 under the reaction conditions, causing a significant drop in HMF yield from 22% to only 9%. The ICP analysis of the reaction mixture showed the leaching of Cu from HUKUST-1, which can be due to the irreversible degradation of the MOF´s structure under hydrothermal conditions.

Acknowledgments
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OC23

Optimizing drug combinations for melanoma therapy by machine learning in zeolite delivery systems

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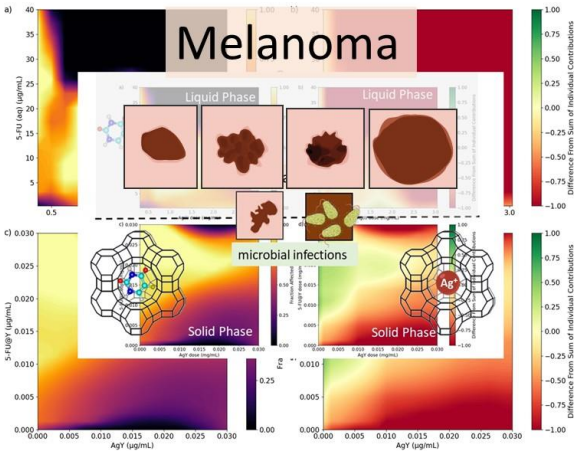
Scientific topic: Medicinal and pharmaceutical applications

Machine learning (ML) models are increasingly recognized as invaluable tools for exploring potential drug combinations[1,2]. Two distinct Artificial Neural Network (ANN) models were used to optimize drug combinations within zeolite-delivery systems (ZDS) for cancer therapy Several ZDS with silver (Ag^+, antimicrobial, and anticancer agent) and 5-Fluorouracil (5-FU, classical antineoplastic agent) were prepared and their characterization confirmed the successful integration of both pharmacologically active components without compromising the zeolite structure. Employing data from the cell viability assays using the A375 melanoma cell line which involved ZDS samples (solid phase) alongside 5-FU and Ag^+ aqueous solutions (liquid phase), two separate ANN models were trained. These models demonstrated high accuracy in predicting experimental cell viability outcomes, facilitating the development of a novel protocol for virtual cell viability assays. Notably, the results indicated that the incorporation of both Ag and 5-FU into the zeolite structure significantly enhanced their anticancer efficacy compared to the liquid phase. Furthermore, two optimal AgY/5-FU@Y ratios (Scheme 1) to achieve the most favourable cell viability outcomes were proposed, providing valuable insights for future drug combination optimization strategies in melanoma therapy[2].



Scheme 1: Schematic representation of the ANN models that were used to determine the optimal drug combination of ZDS for cancer therapy, adapted from[2].

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OC24

Biomass-derived catalysts: heteroatom doping and metal incorporation towards high performance oxygen reduction

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Scientific topic: Electrocatalysis

Electrochemical energy conversion devices such as fuel cells and metal-air batteries have arisen as promising alternatives to fossil fuels combustion. However, both technologies rely on several electrochemical processes, including oxygen reduction reaction (ORR), whose sluggish kinetics and large overpotentials hinders their practical application.[1] These limitations can be overcome by the development of highly effective electrocatalysts.

While currently Pt-based materials are considered the state-of-the-art electrocatalysts towards ORR, heteroatom-doped carbon catalysts arose as promising precious metal-free alternatives.[2] Recently, carbon materials obtained from the pyrolysis of biomass, known as biochars, have attracted interest as highly sustainable catalysts, due to their tunable physical-chemical properties, renewable feedstock, and low production cost.[3] Shrimp shells derived biochars, in particular, have very interesting electrocatalytic properties, originated from the feedstock natural abundance in heteroatoms (e.g. N, S, P).[4]

On the other hand, heteroatom doped-biochars act as excellent supports for other electrocatalytic active species, including transition metals nanoparticles and metal oxides, forming hybrid electrocatalysts with enhanced ORR performance.[3]

Herein, we reported the preparation, physical-chemical characterization and ORR performance of several biochar-based catalysts. The initial biochar, obtained directly from carbonization of shrimp shells, was subjected to heteroatom doping via solventless ball milling under different experimental conditions. Finally, Co or Co_3O_4 nanoparticles were incorporated in our most promising doped-biochar. While all the prepared catalysts showed activity for ORR, both the heteroatom doping and metal incorporation led to enhanced ORR performance, being particularly advantageous in increasing the selectivity for the direct reduction to water (4 electrons route) and lowering the reaction overpotential.

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OC25

Development of waste-based carbon dots as photo-nanocatalysts

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Scientific topic: Photocatalysis

Carbon dots (CDs) are metal-free and carbon-based nanoparticles with a quasi-spherical shape, with sizes typically below 10 nm.[1,2] They possess a core that can be either nano-crystalline or amorphous, and a surface composed by different functional groups (amines, carboxylic acids, hydroxyl groups, etc.) and can be tuned by varying the precursors and synthesis strategies employed.[3]

CDs have been attracting much attention due to their strong photoluminescence, good water solubility, (photo)chemical stability, broadband optical absorption, biocompatibility, low toxicity, and ease of functionalization.[1,2] Furthermore, they show potential for mass production via green bottom-up procedures and for using organic residues as precursors.[4,5] As a result, it is not surprising that they have been investigated in various applications including bioimaging, sensing, photocatalysis and in light-emitting devices, among others.[1-4]

In this work, we aimed to the development of novel CDs to be employed as photo-nanocatalysts.[5,6] More specifically, we have produced them from relevant agricultural waste, such as corn stover, in a circular economy and waste valorization approaches. These nanomaterials were thoroughly characterized by AFM, XPS, XRD, FTIR, UV-Vis and fluorescence spectroscopy. Here, we will demonstrate how they can be used as photocatalysts for the degradation of organic dyes in water samples under visible light irradiation. Namely, photocatalytic nanocomposites were prepared from TiO_2 nanoparticles and the CDs, with the latter enhancing visible light absorption and hindering recombination of photogenerated charge carriers. It will also be shown the enhancing effect of these waste-based CDs to enhance light-emission from marine chemiluminescent reactions.

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OC26

Pd-catalyzed aminocarbonylation continuous-flow process: Multigram synthesis of carboxamides

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Scientific topic: Homogeneous catalysis

Amides are relevant compounds in synthetic, medicinal and biological chemistry. The carboxamide moiety is often present in several fine chemicals and pharmacologically active compounds. Therefore, the development of industrial-scale processes for their preparation is highly desirable.[1] In this regard, the Pd-catalyzed aminocarbonylation reaction stands as a straightforward tool to obtain amides from alkenyl or aryl iodides, carbon monoxide and an amine nucleophile.[2] However, its transition to an industrial scale, offers significant challenges, such as building sizable reactors that offer high yields and the CO gas safe manipulation, which are among the biggest issues.[3] Within this context, there has been increased attention on the transposition of Pd-catalyzed aminocarbonylation reactions from batch to continuous flow chemical processes.[3] This shift offers advantages, resulting from a particular control over reaction parameters, which may lead to higher selectivity and productivity.
In this communication we describe an efficient continuous-flow process that integrates a custom-designed gas input control system, coupled with a tubular reactor for Pd-catalyzed aminocarbonylation of iodoalkenes and iodoarenes, using CO as carbonyl source, and biologically relevant amines as nucleophiles, Figure 1. The implementation of the continuous process and optimization of reaction parameters are presented. The process operates under moderate conditions (CO pressure ≤ 3 bar and T ≤ 100 °C), allowing the multigram scale production of biologically relevant carboxamides, with productivities of up to 20 g/day. Their synthesis, isolation and structural characterization are presented and discussed.

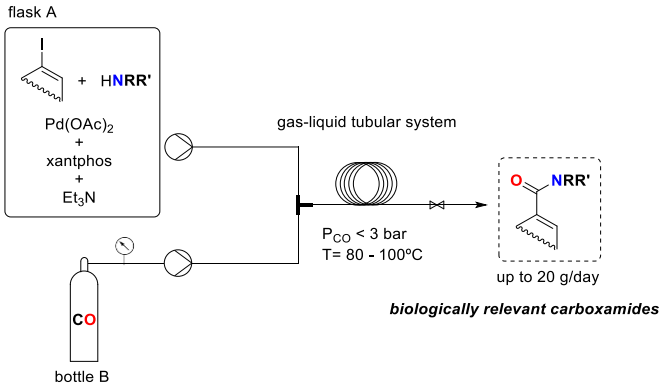

Figure 1: Continuous flow process of carboxamide synthesis via Pd-catalyzed aminocarbonylation.

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OC27

Highly selective phthalocyanine-based catalysts for CO_2 addition reactions to epoxides

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Scientific topic: Homogeneous catalysis

The CO_2 addition reactions to epoxides has sparked significant interest in the scientific community leading to advancements in converting carbon dioxide into valuable chemicals such as cyclic carbonates and polycarbonates, both with relevant applications, namely as green solvents, lubricants, cosmetics, electrolytes in lithium batteries or in plastic engineering, respectively. [1-4] These reactions have been mainly accomplished through the use of metal catalysts, such as complexes of salens, β-diiminates, aminotriphenolates, porphyrins and phthalocyanines. Most of them are known to act as Lewis acids that activate the epoxide, while a nucleophile is usually required as co-catalyst, to promote the epoxide ring opening. When the catalyst and co-catalyst are in the same molecule, it is often denoted by bifunctional catalytic system.[5]
In this regard, the development of new, efficient, and highly selective catalysts for CO_2 addition reaction to epoxides that avoid the use of solvents and additives remain a significant challenge.
In this communication, we describe the sustainable synthesis of two different families of aluminum (III) phthalocyanine catalysts: a bifunctional cationic imidazolyl and a neutral *tert*-butylphenoxy phthalocyanine. We also report their evaluation in CO_2 addition reactions to epoxides, yield selectively cyclic carbonates or polycarbonates (Figure 1). The effects of catalyst, substrate structures, reactions conditions and the use of co-catalyst are described and discussed.

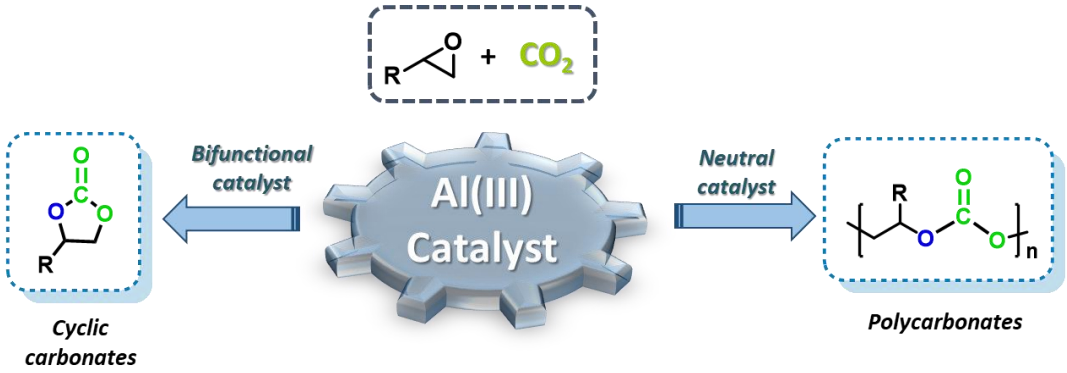

Figure 1: Catalyst modulation for chemoselectivity control in catalytic CO_2 addition reactions to epoxides towards cyclic carbonates versus polycarbonates.

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OC28

Tröger's base–linked POPs as heterogeneous catalysts for the nitroaldol condensation

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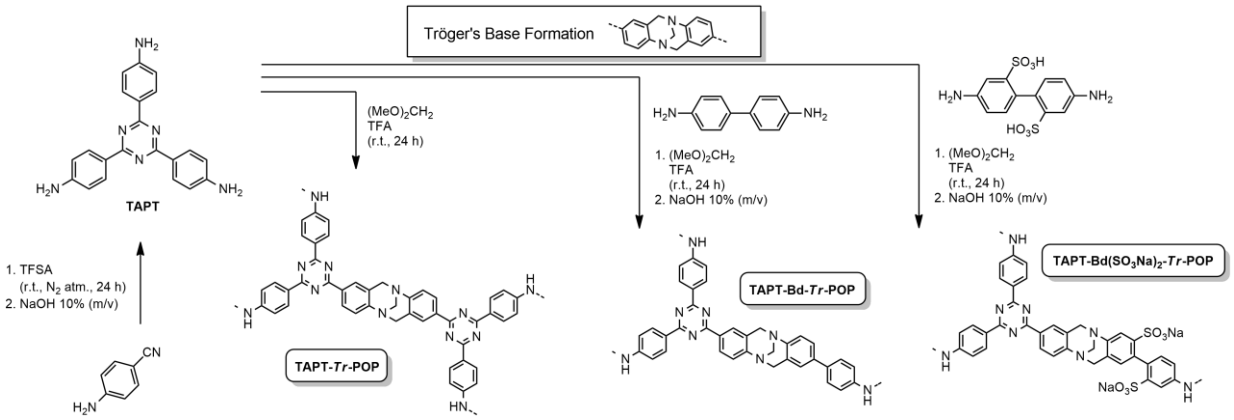
Scientific topic: Preparation of new porous materials; Heterogeneous catalysis

Porous Organic Polymers (POPs)[1] are an exciting class of organic materials, usually prepared from rigid, aromatic monomers containing well-defined structures, exhibiting high degree of reticulation and directional growth in 2D or 3D layers. POPs are known for combining physical properties such as high, permanent porosity, high surface area, high thermal and chemical stabilities, as well as synthetic versatility, allowing for the preparation of highly-specific materials with highly-tunable pore wall functionalization and chemical environment. For these reasons, POPs are potential candidates for a myriad of industrial and technological applications, including heterogeneous catalysis[2]. Tröger's base is a rigid compound, with a V-shaped bridged bicyclic linkage, obtained from the condensation of aromatic amines and a methylene donor, in highly acidic medium. Tröger's base-linked POPs, in particular, are porous, highly crosslinked N-rich materials containing a wide distribution of tertiary amines across the pore walls, making them suitable catalysts for base-promoted reactions.
In this work, three Tröger's base-type POPs have been synthesized, via the condensation[3] of C_3-symmetric 1,3,5-tris(4-aminophenyl)triazine (TAPT) and other amines, to evaluate the effect of pore size and pore wall functionalization on the conversion efficiency towards the Henry nitroaldol reaction. The POPs were characterized by FTIR-ATR, TGA, SEM and BET techniques. Catalytic studies were carried out using nitromethane and benzaldehyde derivatives as substrates.



Scheme 1: Syntheses of Tröger's base–linked POPs.

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OC29

Upgrading of biomass derivatives to biobased products for drop-in-fuels and chemicals over Niobium-based catalysts

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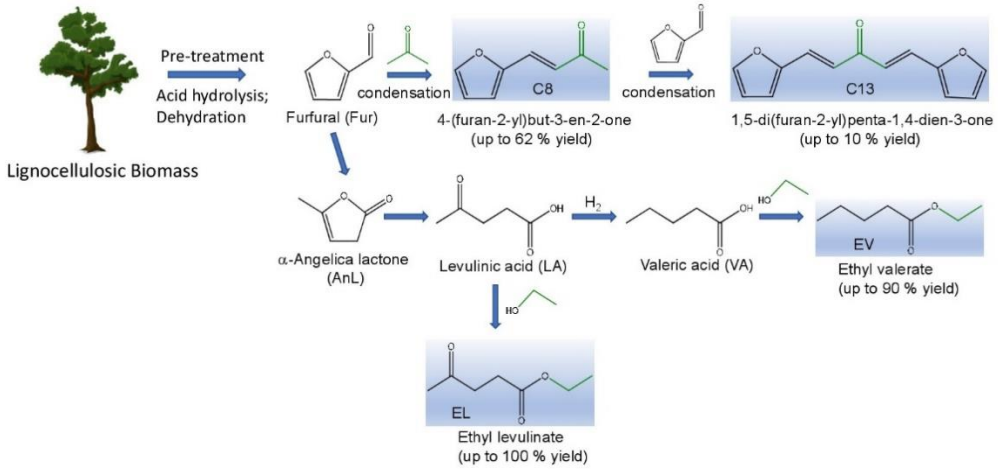
Scientific topic: Heterogeneous catalysis

Vegetable biomass is a potential sustainable alternative to produce renewable products. Carbohydrates are predominant components of biomass, which can be converted via different catalytic routes to a plethora of important chemicals with applications in different industrial sectors. Furfural (Fur) is a recognized industrial platform produced via acid-catalysed conversion of carbohydrates, and its market applications include solvents, polymers, agrochemicals, fuel additives. Important Fur upgrading systems include Fur condensation with acetone which gives intermediates to drop-in-fuels, such as 4-(furan-2-yl)but-3-en-2-one (C8) and 1,5-di(furan-2-yl)penta-1,4-dien-3-one (C13) (Scheme 1). C8 and C13 may be produced via acid or base catalysis, albeit the former may advantageously avoid neutralization steps prior to Fur upgrading. On the other hand, water is a co-product in most biomass conversion processes. In this sense, water tolerant niobium-based oxide catalysts are promising for Fur upgrading. In this work, several reaction systems involving acid catalysis were studied which are related to Fur upgrading over Nb-containing catalysts. Specifically, Fur condensation to C8 and C13, one-pot conversion of □-angelica lactone (AnL) to ethyl levulinate (EL), and esterification of biobased carboxylic acids, namely levulinic acid (LA) and valeric acid (VA) (Scheme 1). Silica-wrapped niobium oxide nanostructured catalysts (*e.g.*, SiNb42) led to yields of up to 62 % C8 from Fur, 90 % EL from AnL and ethyl valerate from LA, and quantitative yield of EL from LA, at 140 ºC.



Scheme 1: Catalytic upgrading of furfural to different biobased products, such as 4-(furan-2-yl)but-3-en-2-one (C8), ethyl levulinate (EL) and ethyl valerate (EV) in the presence of SiNb42.

Acknowledgements
This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIBD/50011/2020, UIDP/50011/2020& LA/P/006/2020, financed by national funds through the FCT/MCTES (PIDDAC). The position held by M. M. A. was funded by national funds (OE), through FC, I.P., in the scope of the framework contract envisaged in the numbers 4, 5 and 6 of article 23 of the Decree-Law 47/2016 of 29 August, changed by Law 57/2017 of 19 July (https://doi.org/10.54499/DL57/2016/CP1482/CT0062).

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OC30

Fruit ripening mitigation – Ag-based-ZSM-5 materials for ethylene removal under competitive adsorption

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Scientific topic: Other applications of porous materials for energy and environment

The EU's fresh and fruit production has been increasing over the years. However, reports show that almost half of the production is simply wasted[1]. Ethylene, a natural fruit hormone that triggers and accelerates the ripening process, is the main responsible[2]. Even though technologies such as controlled atmosphere chambers and ventilation are used to control ethylene levels, traces of ethylene can be found[3]. Adsorption technology is an effective and cheap alternative method. Ag-based zeolite materials, e.g., Ag-ZSM-5, can adsorb lots of ethylene due to the π complexation between Ag^+ species and ethylene[4]. However, other compounds (H_2O, CO_2, VOCs) are also present in the storage chambers and can adsorb competitively with ethylene.

Here, four Ag-ZSM-5 adsorbents were used for their excellent ethylene adsorption capacity: 4Ag-HZSM-5(15), 4Ag-NaZSM-5(40), 6Ag-NaZSM-5(15), and 6Ag-HZSM-5(40) (4-6 wt.% Ag, H^+ or Na^+ as compensating cations and Si/Al ratio of 15 or 40). Details on sample's preparation can be found elsewhere[4]. The four Ag-ZSM-5 adsorbents were tested through breakthrough curves (BC) with binary, tertiary and quaternary mixtures (50 ppm ethylene, 2 % vol. CO_2, 15 ppm ethanol, 80 % relative humidity). The maximum ethylene adsorption capacity was evaluated under those competitive conditions. Ethanol was used as VOC compound. Figure 1 shows the ethylene BC curves for sample 6 Ag-HZSM-5(40) and the ethylene adsorption capacity of all the samples (binary mixtures). The breakthrough curves show that i) water is the major competitor for ethylene adsorption sites since it exhibits a higher affinity towards the ethylene surface[4], ii) ethanol has still a significant effect on ethylene adsorption, though being less polar than water, iii) nonpolar CO_2 molecule does not interact with Ag^+ species and does not compete with ethylene, Comparing the maximum ethylene adsorption capacities for all the samples, we can see that ethanol and water have a higher influence on zeolites with lower Si/Al ratios (more hydrophilic samples). The adsorbents with higher Si/Al ratio present a lower ethylene adsorption (less Ag^+ species present) and also show a smaller reduction of the ethylene adsorption capacity under competitive conditions. Overall, a high Ag content together with high hydrophobicity of the zeolite are the main factors in achieving a high ethylene adsorption capacity under competitive conditions.

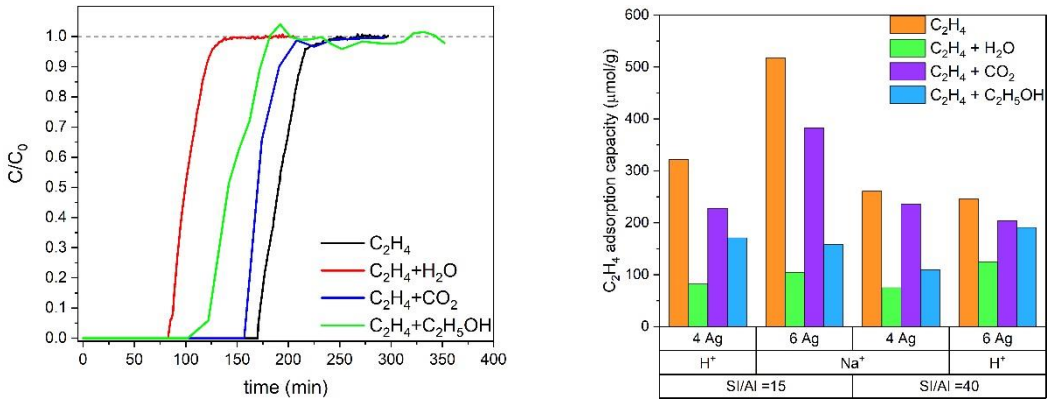

Figure 1: Ethylene competitive adsorption breakthrough curves performed with 6%Ag-HZSM-5 sample (left) and ethylene maximum adsorption capacity for all the samples (right).

Acknowledgments: Nano4fresh (PRIMA/0015/2019); CQE - FCT (UIDB/00100/2020, UIDP/00100/2020 and 2022.12593.BD); IMS - LA/P/0056/2020.

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OC31

Advanced heterogeneous degradation strategies for trimethoprim using porphyrin catalysts: from H_2O_2 treatment to photocatalysis and flow chemistry processes

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Scientific topic: Photocatalysis/Heterogeneous catalysis

The problem of antibiotics' persistence and accumulation in the environment, especially in water systems, stands as a paramount global challenge, due to their status as the most prescribed and used drugs worldwide.[1] Among these antibiotics, trimethoprim (TMP), ranked as the 4th most prescribed worldwide, is frequently identified in water sources due to its recalcitrant nature. Hence, the quest for effective aqueous alternatives to degrade it, such as Advanced Oxidation Processes, becomes imperative.[2]

Herein, we present and discuss our recent findings on the efficient degradation of TMP utilizing three distinct approaches. Briefly, in the first strategy (Figure 1, left), complete degradation of TMP was achieved within 2 hours by employing a stable Mn(III) meso-aryl substituted porphyrin as a catalyst in either a homogeneous or heterogeneous (porphyrin covalently linked to silica) systems, with H_2O_2 serving as a benign oxidant. In a different approach Figure 1, right), a photocatalytic system was implemented and a full TMP degradation was reached in 4 hours, using as photocatalyst a porphyrin encapsulated into an acetylated lignin biopolymer, under aerobic conditions.[4] This system could reach an impressive 75% TOC removal. Finally, a third methodology was used, in which a continuous flow system using as oxidative catalyst a silica immobilized stable Mn(III) porphyrin in a fixed bed reactor and H_2O_2 serving as a benign oxidant, reaching a constant 97% TMP degradation rate during an operational time of 8 hours, with 10 min. residence time, showing TOC values above 75%.

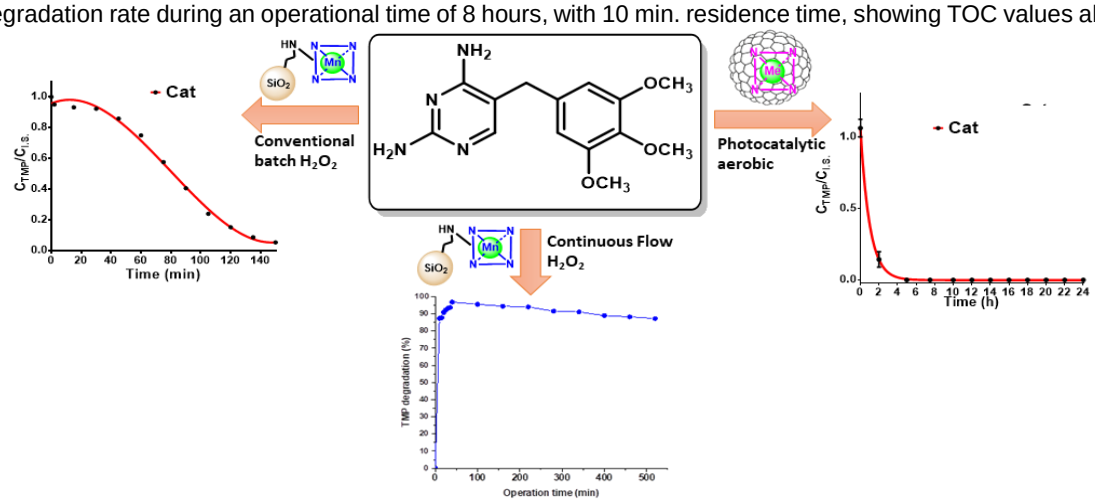

Figure 1: Catalytic pathways for TMP oxidative degradation.

Acknowledgements
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OC32

Getting insights about zeolite desilication through machine learning

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Scientific topic: Heterogeneous Catalysis

Due to their tunable characteristics, zeolites present a wide range of applications, namely in catalysis. Correlating their properties with the preparation conditions through models would speed up the optimization of these materials, avoiding excessive time spent in trial-and-error optimization [1]. However, the physical processes behind the zeolite preparation are very complex which difficult the creation of such models. To solve this problem, a data-driven approach was studied using the initial zeolite properties and the desilication treatment conditions as inputs. The advantage of this technique is that no prior knowledge of the models' structures is required.

Initially a ZSM-5 desilication dataset was created by improving the dataset published by V.Blay *et al.*[2] increasing the dataset from 116 data points to 236 by mining data from literature. To uniformize the data set, only the data points with a desilication procedure using NaOH as a base and without further acid treatment were considered, resulting in a final dataset of 125 data points and 14 variables. The Random Forest Regression (RFR) and Gradient Boosting (GB) models were trained and compared, with GB presenting lower mean squared error in predicting the final zeolite chemical and textural properties on the desilication dataset.

Based on feature importance (see Fig. 1), the Si/Al ratio, BET area and NaOH concentration appeared as the most important input variables, while the temperature and time showed less impact than expected. This can be explained by the low variability of temperature and time in the dataset, being harder for the model to capture their actual importance. However, the partial dependence plots that are used to visualize the correlation and dependence between one output variable and one input variable, showed that the models were still capturing an impact of the temperature and time on the output variables consistent with the experimental studies performed by other authors.

In conclusion, the results demonstrate the effectiveness of employing Machine Learning models in a zeolite post-synthesis to simulate the desilication procedure, serving as a promising starting point. These findings open the zeolite research field to different and more extensive goals.

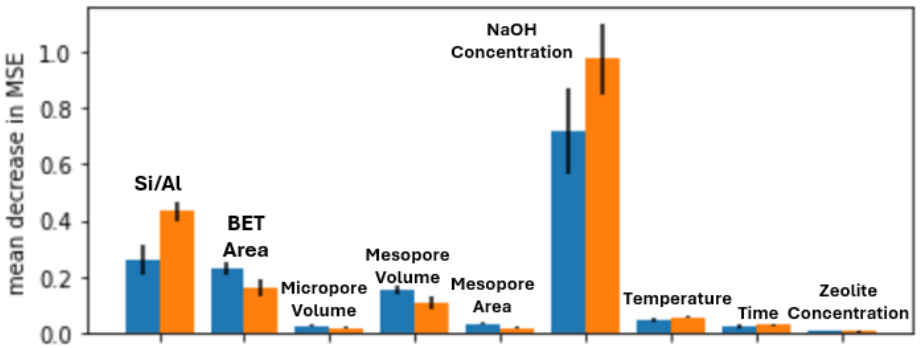

Figure 1: Feature Importance on the final mesopore volume. Legend: **blue** – RFR, **orange** – GB.

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OC33

Improved ethylene production over calcium doped $LaInO_3$ perovskite nanofibers

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Scientific topic: Heterogeneous Catalysis

Ethylene, a vital raw material in petrochemical and in the production of popular plastics such as HDPE and LDPE, presents challenges as its global production depends on steam and thermal cracking of naphtha. [1] Alternative processes for the production of ethylene have been emerging, such as Oxidative Coupling of Methane (OCM), that offers a promising solution. [2] Nitrous oxide (N_2O) emerges also as a potential oxidant for this reaction due to its mild oxidizing tendency that favors the formation of ethylene. [3] Moreover, catalysts development, particularly those with alkaline and rare-earth metals has gathered attention due to its potential to enhance ethylene yields. [4,5] In recent years, perovskites comprising alkaline earth and rare-earth metals emerged has potential catalysts for OCM, which was attributed to their unique physical and chemical properties, namely low vacancy formation energy, high oxygen mobility and high thermal and structural stability.[6,7] The use of rare earths, alkaline earth and other transition metals can produce electronic defects and structural changes, increasing the mobility of oxygens and improving the activation of ethane and, therefore, increasing the OCM activity and selectivity towards ethylene. [4,5] Nanofibers, known for their high surface areas and low-cost production, also demonstrate potential as catalysts but its applications are scarce or inexistent in OCM aiming the production of ethylene. [6,7] Herein, we present the synthesis and characterization of calcium doped $LaInO_3$ perovskite nanofibers and the impact of lanthanum doped perovskites ($La_{1-x}Ca_xInO_3$) and indium doped perovskites ($LaCa_{1-x}In_xO3$) in their OCM catalytic behavior using nitrous oxide as oxidant. The factors that seem to contribute to the differences in activity and selectivity along the different ratios are the catalysts reducibility, crystallite size and acid-base properties (Figure 1). The best results were those obtained over the catalysts with indium dopped by calcium, namely: $LaCa_{0.9}In_{0.1}O_3$ or $LaCa_{0.5}In_{0.5}O_3$.

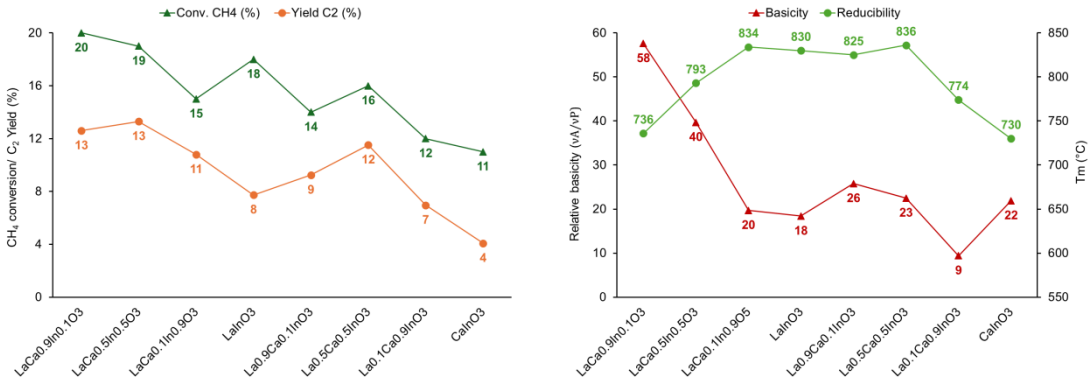

Figure 1: Catalytic behavior of calcium doped LaInO3 perovskite nanofibers: influence of acid-base and redox properties.

Acknowledgements
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POSTER PRESENTATION ABSTRACTS

P1

Functionalized biochars as efficient CO_2 adsorbents and renewable catalysts in cycloaddition to epoxides

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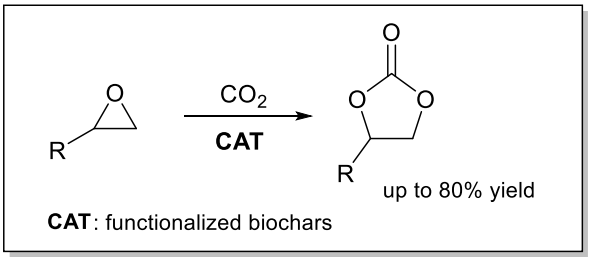
Scientific topics: Preparation of new catalysts and/or porous materials; Heterogeneous catalysis

The use of biomass for preparation of porous carbon materials, such as biochar, is currently a topic with increasing interest for academics and industrials.[1] Besides their low cost, high abundance and stability, biochar materials can be appropriately tailored by different physical and chemical techniques, maintaining their porous structure and surface properties. These are important features that have allowed their efficient use as CO_2 adsorbents and as heterogeneous catalysts in relevant reactions for biomass valorization, namely in carbon dioxide (CO_2) addition reactions to epoxides, aiming at the preparation of cyclic carbonates.[2,3]
Herein, we describe the synthesis and physical/chemical characterization of renewable biochar materials, obtained from pyrolysis of *eucalyptus globulus* wood, an invasive species found in Portuguese forests. Aiming to improve their CO_2 adsorption ability and catalytic activity, differently functionalized carbon materials were prepared, namely N-doped and metal-coated biochars (eg. aluminium, copper, chromium), through physical vapor deposition techniques. The studies of CO_2 adsorption/desorption isotherms are presented to appraise and compare their CO_2 adsorption ability. Furthermore, their application as reusable heterogeneous catalysts in CO_2 addition reaction to epoxides in the absence of any solvent or co-catalyst is described (Scheme 1). The effects of the materials functionalization in their CO_2 adsorption capacity, catalytic activity, selectivity towards cyclic carbonates and recyclability are evaluated and discussed.



Scheme 1: CO_2 cycloaddition reactions to epoxides catalyzed by functionalized biochars.

Acknowledgements
The authors are thankful to Portuguese Agency for Scientific Research “Fundação para a Ciência e a Tecnologia” (FCT) for funding through projects UIDB/00313/2020 and UIDP/00313/2020 to Coimbra Chemistry Centre (CQC). We also acknowledge the University of Coimbra/Santander Universities for funding through Project PT0047.F.02.C (CO2BioFilter).

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P2

Solvent-free acetalization of glycerol using acidic zeolites as heterogeneous catalysts

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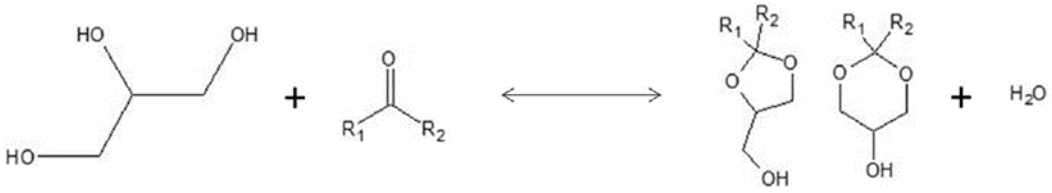
Scientific topic: Heterogeneous catalysis

Fossil fuels have been a great contributor to the current climate crisis. A possible short to medium term alternative to these fuels may be biodiesel.[1] Despite its growth in the last decades, production of biodiesel is still not economically viable in comparison to petrodiesel. In order to improve the economic viability of the whole process, there has been a lot of scientific interest in using glycerol, the major by-product of biodiesel production, as a feedstock for the synthesis of added-value compounds through a variety of pathways. One possibility is the acid catalyzed acetalization reaction for synthesizing alternative fuel additives. Most of the research on this reaction focus on using acetone as a reagent, selectively synthesizing (2,2-dimethyl-1,3-dioxolan-4-yl)methanol, also known as solketal, but other aldehydes and ketones also react in the same way and the resulting products also show potential as fuel additives.[2,3] In this work, we will present our current approach in optimizing the acetalization of glycerol with alternative ketones and aldehydes, utilizing zeolites as heterogeneous catalysts (Scheme 1). The impact of reaction parameters such as the reagent/glycerol molar ratio, reaction temperature, reaction time and catalyst percentage will be highlighted. Glycerol conversion and products' selectivity are determined based on gas chromatography (GC) analyses. The recovery, stability, and reusability of the catalysts will be presented also.



Scheme 1: Acetalization of glycerol under heterogeneous conditions

Acknowledgements
This work received financial support from PT national funds (FCT/MCTES) through LAQV-REQUIMTE (UIDB/50006/2020 & UIDP/50006/2020) and CICECO-Aveiro Institute of Materials (UIDB/50011/2020 & UIDP/50011/2020). The position held by I.C.M.S.S.-V. (Ref. 197_97_ARH-2018) was funded by national funds (OE), through FCT, I.P., in the scope of the framework contract foreseen in the numbers 4, 5 and 6 of article 23 of the Decree-Law 57/2016 of 29 August, changed by Law 57/2017 of 19 July. The NMR spectrometers are part of the National NMR Network (PTNMR) and are partially supported by Infrastructure Project 022161 (cofinanced by FEDER through COMPETE 2020, POCI and PORL and FCT through PIDDAC.

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P3

Composite silica/polymer membranes for catalytic application in biorefinery

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Scientific topic: Heterogeneous catalysis

Biomass stands as a valuable resource for chemicals and products, offering an eco-friendly alternative to those derived from fossil fuels. Finding routes of valorization and transformation of biomass platform molecules like levulinic acid or furfural holds immense potential for driving renewable chemical processes within the Biorefinery framework. Sustainable progress in developing heterogeneous catalysts is pivotal for realizing this objective.[1] Moreover, as we transition towards a circular bioeconomy and strive for commercially viable biorefineries that are both environmentally sound and economically viable, a key strategy involves maximizing the value of all biomass components and products. Within this context, the adoption of advanced technologies such as membrane reactors is crucial for process intensification.
In this study, we developed two categories of catalytic membranes composed of composite materials. One set employed PVA as the polymer matrix, while the other utilized Polymer with Intrinsic Porosity (PIM). These matrixes were combined with two distinct types of solid porous catalysts, modified MCM41 and SBA 15, to form the membranes.
Mesoporous silica stands out as an attractive material owing to its exceptional thermal and chemical stability. The mesoporous surface can be graft with acid sites through chemical functionalization.[2] In this study, alkyl sulfonic acid functionalization of this inorganic support was employed to produce solid catalysts.
Composite membranes underwent preparation and optimization via various procedures, exploring the impact of parameters like catalyst loading, solvent used, and the addition of a cross-linker. This approach yielded materials exhibiting homogeneity with well-dispersed catalytic phases. Subsequent characterization and study of these membranes were conducted in the furfural acetalization reaction.

Acknowledgements
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P4

Shrimp shells derived Pd/N-doped biochar for (electro)catalytic applications

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Scientific topic: Heterogeneous catalysis

Biochar has arisen as a promising alternative to conventional carbon materials. Its renewable feedstock origin and low production cost makes it a more sustainable option than fossil fuel derived materials. The chemical composition, morphology and physical-chemical properties of biochar are reportedly dependent on the choice of the biomass feedstock [1]. Crustacean shells are rich in chitin, a biopolymer containing a high content of nitrogen, proteins and minerals such as $CaCO_3$, containing also small amounts of sulphur and phosphorus [2]. This composition is extremely beneficial to biochar production: heteroatoms are mostly preserved during the synthesis and $CaCO_3$ can act as self-template leading to the formation of highly porous structures.
In this work, shrimp shells-derived biochar were prepared through pyrolysis and N-doping (using urea as nitrogen source) *via* ball milling mechanical activation. The resulting N-doped carbon has been used as support for palladium immobilization by wet impregnation approach (Pd/N-BCH). The versatility of the obtained material was then successfully demonstrated in: a) catalytic aminocarbonylation of haloarenes for the synthesis of aromatic amides [3]; and, b) energy-related electrochemical processes: hydrogen reduction reaction (HER) and oxygen reduction reaction (ORR), both critical parts in energy conversion devices (e.g. fuel cells and metal-air batteries) [4]. Pd/N-BCH achieved a E_{onset} of 0.81 V vs. RHE and j_L of -3.70 mA cm^{-2} for ORR, as well as good selectivity for the direct reduction to water; in HER, it showed a η_{10} of only 274 mV. In the catalytic aminocarbonylation of iodobenzene, the Pd/N-BCH catalyst, showed high activity and selectivity, with up to a 99% conversion and full selectivity for the carboxamide product, when xantphos was used as P ligand. In the absence of any P ligand, the catalyst presented moderate activity (30% conversion) achieving both carboxamide (ca. 55%) and ketoamide product (ca. 45%). Here in we will present versatile N-doped Pd-supported biochar with great potential for (electro)catalytic processes..

Funding
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Acknowledgements
This work received support and help from FCT/MCTES: UIDP/50006/2020 DOI 10.54499/UIDP/50006/2020 and UIDB/50006/2020 DOI 10.54499/UIDB/50006/2020), through national funds; R.M. PhD fellowship 2020.05342.BD. D.M.F. and A.F.P. through the Individual Call to Scientific Employment Stimulus (Refs. 2021.00771.CEECIND/CP1662/CT0007 and 2020.01614.CEECIND/CP1596/CT0007, respectively). V.M. thanks the fellowship in the project EXPL/BII-BIO/0436/2021.

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P5

C-scorpionate Cu(II) complexes immobilized at HZSM-5 zeolite as efficient catalysts for hydrocarbon and alcohol oxidations

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Scientific topic: Heterogeneous catalysis

Currently, the industrial oxidation of hydrocarbons and alcohols to high-added-value products is typically performed under high temperatures and pressures. The increased concerns regarding climate and energy crisis, call forth researchers to search for sustainable efficient catalytic processes. However, addressing such needs remains a great challenge.

The knowledge that C-scorpionate metal complexes are capable to act as homogeneous catalysts for the oxidation of cycloalkanes and secondary alcohols under mild conditions,[1-3] prompted us to investigate the use of this type of metal complexes as catalysts for the oxidation of aromatic hydrocarbons and primary alcohols.

In this study, the C-scorpionate copper(II) complexes $[Cu(SO_4)\{HC(pz)_3\}]$ (**1**), $[Cu\{HC(pz)_3\}_2](NO_3)_2$ (**2**) and $[\{Cu(CH_3COO)_2\}_3\{HC(pz)_3\}_2]$ **(3)** (Figure 1a) were immobilized onto different forms of HZSM-5, and their catalytic activity evaluated for the selective oxidations of toluene and of benzyl alcohol to benzaldehyde (Figure 1b) under mild conditions (temperature below 80 °C, green oxidant, solvent-free or green solvents). The influence of reaction parameters, such as time, type and amount of catalyst, temperature, and stability/reusability of the catalyst, are presented and discussed.

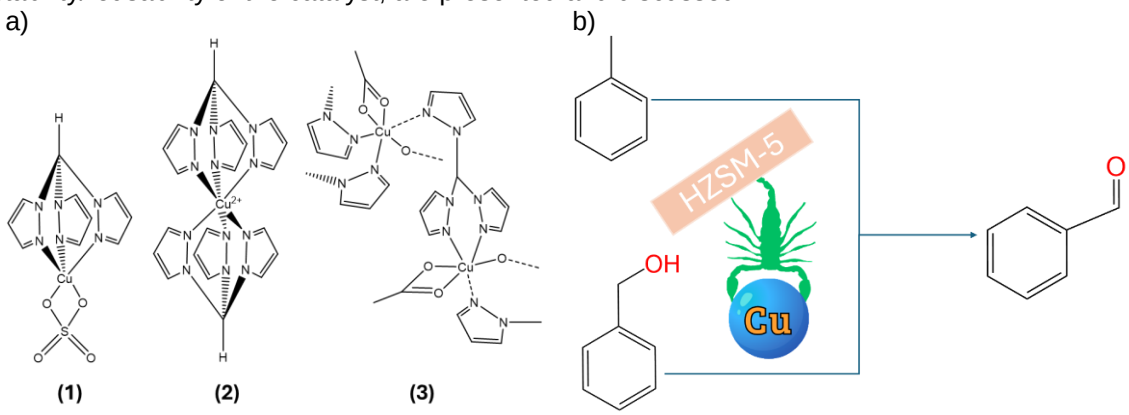

Figure 1: a) Structures of the C-scorpionate copper(II) complexes **1**-**3**. b) Oxidation of toluene and benzyl alcohol to benzaldehyde in the presence of a HZSM-5 heterogenized C-scorpionate Cu(II) complex.

Acknowledgments

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P6

Enhancing the oxidation of alcohols with Fe_3O_4 and $BaTiO_3$ nanocomposites via diverse energy inputs

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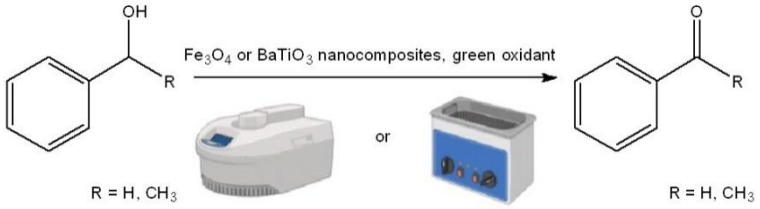
Scientific topic: Heterogeneous Catalysis

Catalysis plays a pivotal role in advancing green chemistry by enabling efficient and sustainable chemical transformations. In this work were explored the synergistic relationship between heterogeneous catalysts, green chemistry principles, and innovative energy inputs such as ultrasound and microwave irradiation and focusing on the oxidation of alcohols, specifically benzyl alcohol and 1-phenylethanol (Scheme 1).
The oxidation of primary and secondary alcohols is a significant transformation in organic synthesis. Benzaldehyde and acetophenone, products of the oxidation of benzyl alcohol and 1-phenylethanol, respectively, are versatile compounds with broad industrial applications, particularly in dyes, perfumes, and pharmaceuticals.[1,2]
Barium titanate ($BaTiO_3$) and magnetite (Fe_3O_4) emerge as promising materials for various energy inputs due to their unique properties. $BaTiO_3$ exhibits ferroelectric, piezoelectric, and dielectric behaviors, while iron oxide demonstrates ferromagnetism.[3,4]
The utilization of heterogeneous catalysts, such as nanocomposites based in Fe_3O_4 and $BaTiO_3$, in green chemistry aims to minimize waste generation, energy consumption, and overall environmental footprint. By employing these catalysts, chemical reactions can be optimized to achieve higher yields and selectivity under milder conditions. Incorporating alternative energy sources like ultrasound and microwave irradiation further enhances the efficiency of catalytic processes by promoting rapid heating. The catalytic peroxidative oxidation of benzyl alcohol, catalyzed by the nanocomposite $BaTiO_3$@Cu_3BTC_2 and enhanced by ultrasound irradiation, achieved an impressive yield of *ca.* 20%, with a remarkable selectivity to benzaldehyde reaching 98% at room temperature. This performance was accomplished with a molar ratio of 2:1 (oxidant:substrate), using acetonitrile as solvent, and employing 5 mg of catalyst over a reaction period of 1 hour. Similarly, the oxidation of 1-phenylethanol yielded a substantial 40% of acetophenone using the nanocomposite Fe_3O_4@Cu_3BTC_2 under microwave irradiation at 80 ºC, 60 W. This reaction also employed a molar ratio of 2:1 (oxidant:substrate), acetonitrile as solvent, and 5 mg of catalyst over a shorter reaction time of 30 minutes.



Scheme 1: Microwave or ultrasound irradiation assisted peroxidative oxidation of benzyl alcohols using Fe_3O_4 and $BaTiO_3$ nananocomposites as heterogeneous catalysts.

Acknowledgements
We thank the Fundação para a Ciência e Tecnologia through projects UIDB/00100/2020, UIDP/00100/2020, and 10.54499/2022.02069.PTDC (http://doi.org/10.54499/2022.02069.PTDC), and by the Instituto Politécnico de Lisboa with the IPL/IDI&CA2023/SMARTCAT_ISEL project. LMMC is also grateful for the Ph.D. grant UI/BD/152790/2022.

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P7

Fenton-like oxidation of drugs with bimetallic-zeolite catalysts

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Scientific topic: Heterogeneous catalysis

Among the numerous drugs found in water sources, one compound that particularly stands out is 4-nitro-2-phenoxymethanesulfonanilide, commonly known as nimesulide. This compound is an Active Pharmaceutical Ingredient that belongs to the non-steroidal anti-inflammatory drugs, renowned for their analgesic, antipyretic, and anti-inflammatory properties. It is widely recognized that the vast majority of these drugs exhibit high stability and resistance to microbial degradation. Advanced oxidation processes (AOPs) have proven to be highly effective in the degradation of organic pollutants present in wastewater due to their oxidation by the hydroxyl radicals formed, offering rapid treatment times and achieving significant performances. The heterogeneous Fenton process has received much attention for its low cost, high efficiency, and moderate operation conditions.[1] This work reports the preparation of bimetallic-zeolite catalysts based in NaY with Fe/Zn, Fe/Co, Fe/Cu and Fe/Ni by the ion-exchange method.[2] Different characterization techniques show that the metals are cationic and show high oxidation efficiency against the drug. The Fe/Co supported in NaY - (CoFe)NaY - catalyst was shown to be more efficient – see Figure 1. A parametric study was then performed with such material, and total nimesulide removal and high mineralization (~87%) were reached when the Fenton process was operated under the best conditions found (t = 120 min, T = 50 ºC, pH_0 = 3.0, [catalyst] = 0.5 g/L and $[H_2O_2]_0$ = 100 mg/L). The (CoFe)NaY catalyst can be used at least five times without a significant loss of catalytic activity.

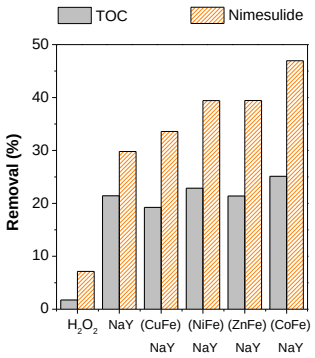

Figure 1: Nimesulide and TOC removal by hydrogen peroxide alone and combined with NaY and by the heterogeneous Fenton process catalyzed with different catalysts (t = 120 min, pH = 5.7, T = 26 ºC, [catalyst] = 0.2 g/L and $[H_2O_2]$ = 100 mg/L).

Acknowledgements
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P8

Hybrid multi-core shell nanoparticles for catalytic wet peroxide oxidation: effect of aqueous matrix

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Scientific topic: Heterogeneous catalysis

Increased complexity, production, and consumption of emerging chemical compounds (such as personal care products, pharmaceuticals, pesticides, and hormones) is creating a significant impact on water quality. It is well known that wastewater treatment plants lack the ability to deal with those compounds. Catalytic wet peroxide oxidation (CWPO) arises as a suitable option to remove micropollutants; and the bottleneck in CWPO is catalyst development. In this work, cobalt ferrite nanoparticles were synthesized and coated with a phloroglucinol/glyoxylic acid resin, followed by pyrolysis to yield a carbon-coated cobalt ferrite particle named CoFe@C_{PG}, as reported elsewhere[1]. CoFe@C_{PG} was applied in the CWPO of paracetamol (PCM) ([PCM] = 100 mg L^{-1}, [H_2O_2] = 474 mg L^{-1}, 80 °C, pH = 3.5, [cat] = 2.5 g L^{-1}) considering different water matrix (ultrapure water, bottled water, hospital wastewater, and river water). The results for PCM and H_2O_2 conversion after 2 h of reaction are depicted in Figure 1. As can be seen, the aqueous media greatly influences the removal of PCM, likely ascribed to the presence of radical scavengers or other compounds that compete for the active center of the catalyst. Nevertheless, in all matrices, complete PCM conversion was obtained with the developed catalyst after 6 h of reaction, and total organic carbon (TOC) removal was higher than 55% in all matrices after 8 h of reaction.

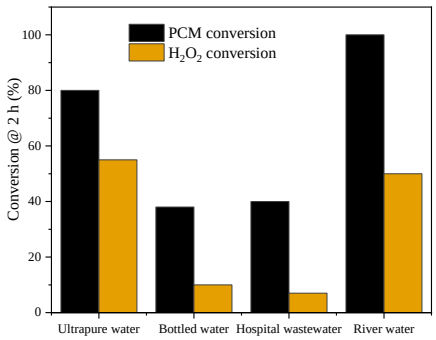

Figure 1: CWPO of PCM considering different aqueous matrices.

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P9

Bulky olefin epoxidation under mild conditions over Mo-based oxide catalysts

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Scientific topic: Heterogeneous Catalysis

The chemical valorisation of olefins via epoxidation (EPO) routes is of great industrial relevance once the epoxides are important intermediates to many end use industries. While homogeneous Mo-based catalytic technologies reached industrial implementation for olefin EPO, since the catalytic EPO process claimed by Halcon International Inc. (USA, 1960), the same doesn't apply for heterogeneous Mo based ones, which continue of great interest, albeit challenging. In this work, the challenge of developing selective and stable epoxidation solid catalysts for EPO of relatively bulky olefins with *tert*-butylhydroperoxide (TBHP) under mild conditions was studied by developing nanocatalysts consisting of Mo and M = Ta, Nb or W oxides prepared via a simple and versatile non-aqueous sol–gel synthesis.[1] The influence of the material synthesis conditions on the material properties was investigated to meet superior catalytic performances.[1] The best-performing catalysts were explored for the EPO of the biobased fatty acid methyl esters (FAMEs), methyl oleate (MO) and methyl linoleate (ML). Mo(75D)M-0.3 with M = Ta, Nb and W (synthesis time of 0.3 h, using 75 at% Mo relative to M, and MoO2Cl2 as precursor) led to 84-95 % and 97-100 % MO and ML conversion, respectively, giving the corresponding epoxides in yields greater than 80 %, at 24 h (Figure 1).1 Exceptionally, the system ML/Mo(75D)Nb-0.3 led to furan type products in 52 % yield. To the best of our knowledge, these are the first Mo,M oxides reported for these reactions.

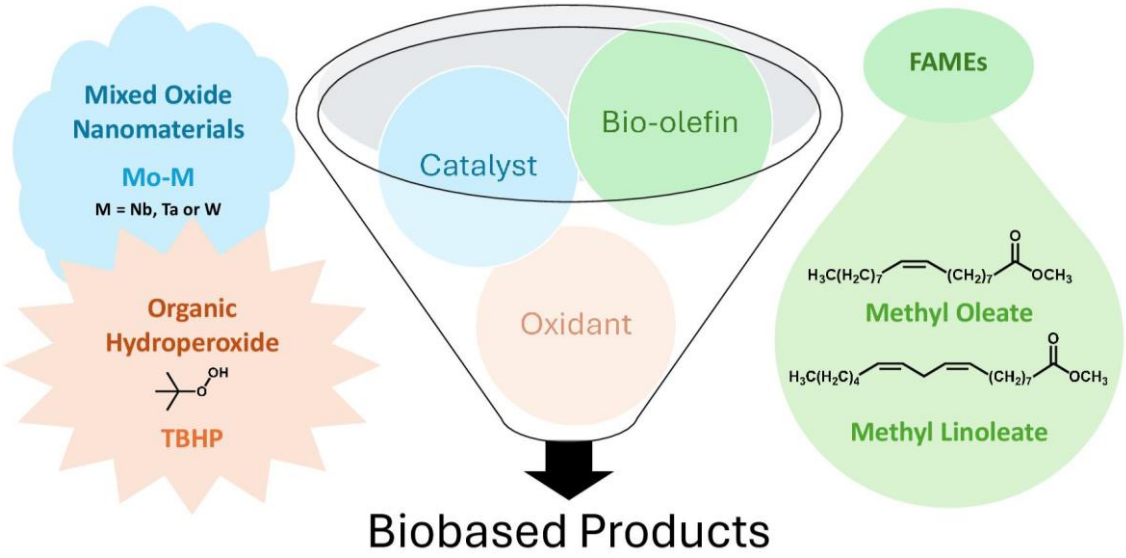

Figure 1: Mixed oxide nanomaterials for bio-olefin epoxidation catalytic systems.

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P10

Surfactant templated hierarchical Pt/Y for the transformation of biomass model compounds through HDO reaction

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Scientific topic: Heterogeneous catalysis

Zeolites have been studied as acidic supports to produce bifunctional catalysts in hydrodeoxygenation (HDO) reaction, a catalytic route to transform oxygen rich biomass-based compounds into biofuels[1]. Catalytic HDO occurs in the presence of bifunctional catalyst, comprising a metal function dispersed on a support with adequate acid and textural properties. The transformation of voluminous compounds can be compromised due to the intrinsic microporous nature of zeolites, so, the use of hierarchical zeolites produced by post-synthesis methods can be a promising solution. In this study, Y zeolite (Zeolyst, Si/Al=5.4) was submitted to an alkaline treatment with NaOH in the presence of CTAB (C) surfactant. In some cases, NaBr (0.1 to 0.7% (w/w)) was added to study the effect of the ionic strength. The zeolite suspensions were kept under autogenous pressure at 150 ºC, for 6 or 24 h. The metal function (1 wt. % in Pt) was introduced by incipient wetness impregnation (IWI) using $Pt(NH_3)_4Cl_2 \cdot xH_2O$ as metal precursor, followed by calcination and reduction under H_2 flow at 450 ºC. The samples were characterized by powder X-ray diffraction, N_2 adsorption isotherms at -196 ºC and TEM microscopy. Figure 1 shows the effect of treatment duration (6 or 24 h) as well as the influence of NaBr addition (0.23% (w/w)) on the textural properties of the hierarchical zeolites.

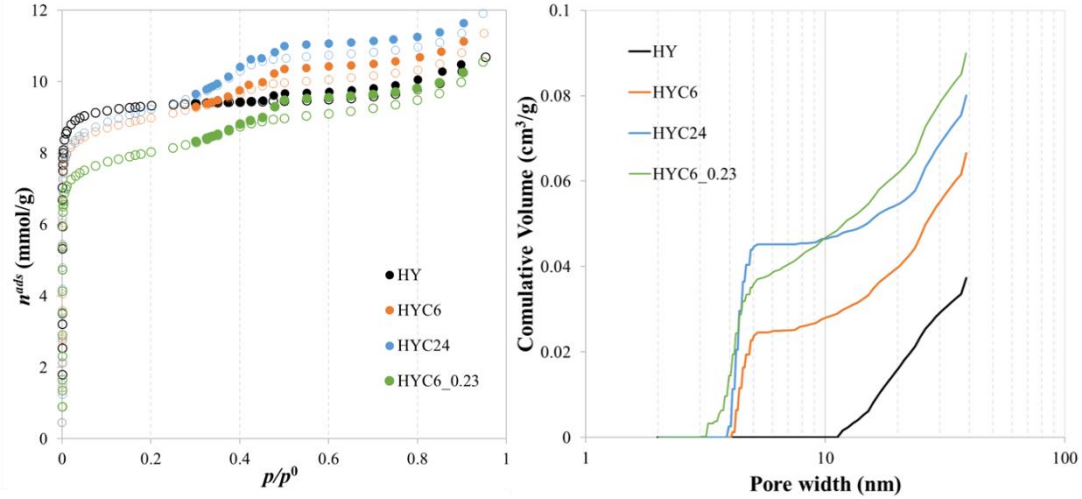

Figure 1: N_2 adsorption isotherms at -196º C (left) and mesopore size distribution (right) for parent and treated with NaOH + CTAB samples treated for 6 and 24 h and NaOH+CTAB+0.05NaBr for 6 h.

As can be observed, the alkaline treatment in the presence of CTAB led to the formation of narrow mesopores (4-5 nm). The presence of NaBr slightly shifts the mesopore range to lower values probably because the increase in ionic strength changes the shape of the micelles.[2] The catalytic behavior of Pt loaded samples on HDO reaction aims to evaluate the effect of the textural modification of the zeolitic support using as reactants two molecules with distinct sizes: anisole and dibenzofuran using a high-pressure Parr reactor at 250 ºC, 20 atm and 350 rpm stirring.

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P11

A green photocatalytic approach to obtain oxidative derivatives of abietic acid

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Scientific topic: Photocatalysis

The use of renewable sources, allied with clean technologies and green chemical processing, including the use of catalysts and photocatalysts, is an interesting approach for a sustainable production of value-added chemicals.
Abietic acid is a natural tricyclic diterpenoid resin acid isolated from pine rosin and can be used as a chemical scaffold to produce valuable chemicals with potential applications namely for medicine and agriculture. These abietic acid derivatives have been shown to exhibit promising anticancer, antimicrobial, antiviral, antiulcer, insecticidal, and herbicidal activities.[1,2]
Knowing that chlorophylls are considered efficient photocatalysts due to their ability to generate oxygen singlet,[3,4] in this study, it was evaluated their potential in the oxidation of abietic acid.
The results showed that abietic acid can be efficiently oxidized under environmentally friendly conditions in the presence of chlorophylls as natural photocatalysts. The best conditions for the photooxidation process to occur such as the photocatalyst/subtract ratio, reaction time and exposure to light will be presented. Additionally, the products obtained and the photocatalyst stability over time will be also subject to discussion.

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P12

Porous Ti-MOF for the hydrogen sulfide adsorption

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Scientific topic: Medicinal and pharmaceutical applications.

Hydrogen sulfide (H_2S) molecule induces several biological effects when delivered exogenously, such as anti-inflammatory, anti-tumor effects, promotion of ion channel regulation, cardio, and neuroprotective effects, vaso-relaxing, and antioxidant. These results led to the research on the possibility of H_2S being used in the treatment of several pathologies [1]. Nevertheless, because it is a gas, H_2S demands new forms of administration that enable control of the location, dosage, and timing of delivery. Within this context, nanoporous materials that can store and release H_2S in controlled ways are of interest for therapeutic applications.
In this work, the MIP-177, a titanium-based metal-organic framework-MOF, was used as an adsorbent material for H_2S storage and release. This MOF previously demonstrated interesting properties for the tunning of cellular responses with the controlled release of nitric oxide [2]. The amounts of hydrogen sulfide adsorbed were evaluated by a volumetric method.

Acknowledgments
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P13

Controlled dual release of NO and H_2S from a porous Ti-MOF for therapeutic applications

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Scientific topic: Medicinal and pharmaceutical applications

Nitric oxide (NO) and hydrogen sulfide (H_2S) are two gasotransmitters within the human body extensively studied. They play crucial roles in several physiological processes, including vasodilation, angiogenesis, immune and inflammatory responses, neurotransmission, apoptosis, and regulation of gene transcription.[1,2] This broad spectrum of functions prompted the intense research for vehicles to target deliver these gases at controlled rates, and for predetermined durations, as a potential treatment for medical conditions where exogenous delivery therapy may be beneficial to supplement or regulate local NO and H_2S levels.

Although current knowledge indicates that cooperation between NO and H_2S signaling pathways is essential for many of their shared physiological roles, the development of porous materials for the simultaneous release of these gasotransmitters is still in a primordial stage of study, since most research efforts focus on singular gas delivery. To this end, we propose a titanium-based metal-organic framework (MOF), named MIP-177, as a potential dual carrier for NO and H_2S. The material's characterization and NO adsorption/release capacity for therapeutic applications have already been documented.[3] Currently, the first studies are underway to assess the extent of H_2S release and its added effects on the overall gas adsorption (H_2S and NO) and delivery potential. Release studies were performed at physiological pH using a phosphate buffer, with H_2S and NO concentrations quantified via DTNB (5,5′ -Dithiobis (2-Nitrobenzoic Acid)) assay (Figure 1. a), and Griess assay (Figure 1. b), respectively.

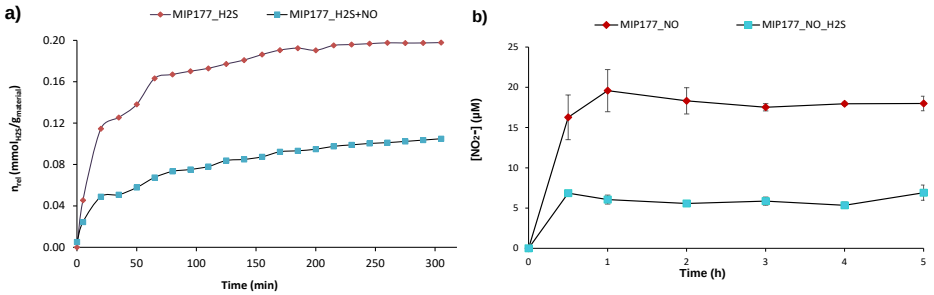

Figure 1: a) H_2S release measured in DTNB assay in the presence of 3 mg of NO-loaded and NO-H_2S-loaded MIP-177; **b)** Nitrite release levels from NO-loaded and NO-H_2S-loaded MIP-177 in a phosphate buffer, at a concentration of 450 µg/mL, quantified with the Griess reagent assay (error represents the standard deviation of n=3).

Acknowledgments
This research was financed by Fundação para a Ciência e a Tecnologia (FCT) in the scope of the projects UIDB/00100/2020 (CQE), UIDB/04028/2020 (CQE), UIDB/04028/2020, and UIDP/04028/2020 (CERENA), and the Institute of Molecular Sciences (IMS) Associate Laboratory funded by FCT through project LA/P/0056/2020 and the project 2022.05605.PTDC (DOI 10.54499/2022.05605.PTDC)

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P14

Asymmetric catalytic multicomponent synthesis of chiral spiro-oxindoles-hydantoins for leishmaniasis treatment

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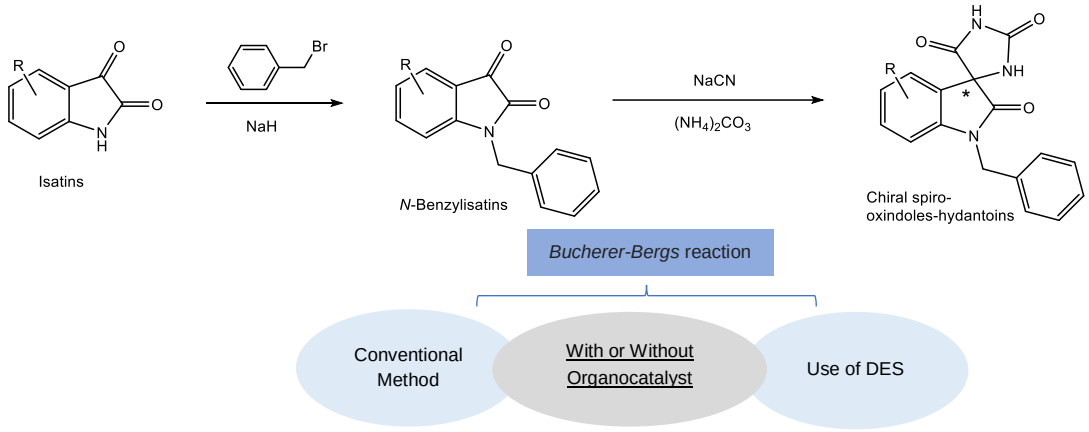
Scientific topic: Medicinal and pharmaceutical applications

Leishmaniasis is a neglected tropical disease (NTDs), being the second biggest cause of death for a parasitic disease in, after malaria.[1] According to the World Health Organization, it is estimated that 700,000 to 1 million new cases are reported every year. Current treatments include antimony compounds, amphotericin B, pentamidine, miltefosine, among others.[2] However, these pharmaceuticals show toxicity, required prolonged usage and are expensive.[3]

Interestingly, several spiro compounds have already demonstrated antileishmanial activity.[4] The oxindole unit is a well-known pharmacophore [5] and, in fact, compounds containing oxindole have been reported for their antileishmanial activity.[6] Hydantoins (imidazolidine-2,4-ones) are also biologically active.[7] In this communication we will discuss our latest results on the multicomponent synthesis (*Bucherer-Bergs* reaction) of a library of spiro-oxindole-hydantoins using Deep Eutectic Solvents (DESs) in the presence of various organocatalysts (**Scheme 1**).

We are currently evaluating these compounds for their antileishmanial activity.



Scheme 1: Synthesis of Chiral spiro-oxindoles-hydantoins.

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P15

Machine learning prediction of the potential of MXenes for catalyzing the water gas shift reaction

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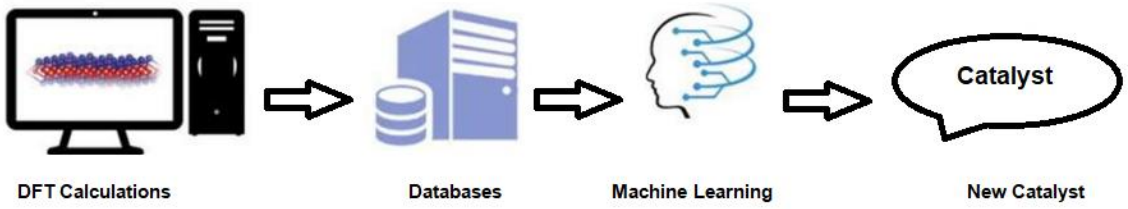
Scientific topic: Theory and Other application(s)

Developing catalysts is crucial for reactions such as the water gas shift (WGS), and machine learning (ML) has become a well-established concept in the chemical sciences. In fact, MXenes, two-dimensional few-layered transition-metal nitrides and carbides, with general formula $M_{n+1}X_nT_x$ (M is an early transition metal, *n* = 1-4, X is C and/or N and T*x* is the surface termination)[1-3], possess substantial surface areas and distinctive physicochemical features, which make them interesting for applications in areas as waste water treatment, energy storage, gas sensing or catalysis.[4] In this work, ML tools are now being utilized to predict the potential of MXenes, based on data obtained from density functional theory (DFT) calculations or sourced from online databases. This facilitates the innovative design of catalysts for WGS. We present the recent research from our group where ML was employed to predict adsorption energies for different species on MXene surfaces, such as H_2O, CO_2, and H_2, and resulting species from their reactivity on the surface.



Scheme 1: Workflow for Catalyst Design Using DFT and Machine Learning for MXenes.

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P16

Sustainable reductive electrochemical amination with metal N-doped biochar electrocatalysts

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Scientific topic: Electrocatalysis

Industry is driving forces to shift chemical production from conventional fossil resources to renewable biomass in order to address the challenge of a 2030 world that leads societal concerns over climate change[1]. Amines are nitrogen-containing chemical compounds that are widely used as essential building blocks for agrochemicals, medicines, and polymers. Currently, hazardous and/or costly chemicals are used in the industrial production of amines from petrochemical resources. This work seeks to advance the state-of-the-art through the development of Electrochemical Reductive Amination (ERA), a clean, safe, affordable, and scalable catalytic process for the production of bioamines from renewable resources. ERA is a substitute for traditional chemical reductive amination that uses only protons and electrons instead of molecular H_2 derived from fossil fuels[2].
Within carbon materials, biochars obtained from available biowaste feedstocks are becoming promising candidates as sustainable carbon materials with potential application in different areas due to their easily tuned surface chemistry and porosity and also renewable feedstock and low production cost[3,4].
In the present study, agroforestry wastes or shrimp shells were pyrolyzed under various conditions to produce porous biochars, which were then doped with nitrogen using either ball milling or wet impregnation. Additionally, different transition metals were used to functionalize the doped biochars. Through chemical/physical experimental conditions, high surface areas (BET > 200 m^2/g) could be obtained through activation, and the success of all functionalization could be observed using XPS, XRD, RAMAN and SEM/EDS. The results of XPS revealed the presence of N-functionalization, and SEM revealed the formation of highly porous structures[5]. The as produced biochars are a promising strategy to improve ERA potential. All the catalytic results and the catalysts performance will be discussed according to the characterization results.

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P17

Copper(II) porphyrin complexes bearing *N*-electron-donating groups as catalysts in the mild oxidation of cycloalkanes

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Scientific topic: Homogeneous catalysis

Metalloporphyrins are well-recognized models of cytochrome P450 enzymes, capable of oxidizing a wide range of organic compounds including saturated hydrocarbons.1 Most of these studies have been carried out with porphyrins bearing electron-withdrawing or bulky substituents at the *meso*-phenyl rings of the macrocycle and using Fe(III) and Mn(III) complexes. Copper is another metal that plays an important role in biological catalytic systems due to its bioavailability, presence in active sites of oxidizing enzymes and a rich redox and coordination chemistry. However, with regard to catalysis by porphyrin derivatives, much less attention has been given to the development of Cu-based catalytic systems.2
With this motivation and our interest in both metalloporphyrin chemistry and oxidation catalysis with copper systems, in the present work, we discuss the synthetic approaches for the preparation of novel copper(II) complexes of porphyrins bearing bulky and *N*-electron-donating groups at *meso*-positions, followed by the exploration of their catalytic activity in the mild oxidation of different cycloalkanes to the corresponding cyclic alcohols and ketones.

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P18

A perovskite-based three-dimensional particulate electrode for water carbamazepine removal

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Scientific topic: Electrocatalysis

This research presents an innovative approach for removing carbamazepine (CBZ), a persistent pharmaceutical contaminant, using a three-dimensional electro-Fenton (TDEF) system. The preliminary phase involved validating the configuration of the TDEF reactor. First, commercial electrodes, metal-mixed oxide as the anode, and stainless steel as the cathode were selected. After that, a third particulate electrode with electrocatalytic capacity was introduced, working with two options: vineyard biochar and a lab-made conglomerate of perovskite and carbon black. Additionally, two collector systems were evaluated for easy recovery and reuse of this three-dimensional particulate electrode: a thermoplastic tube and a silicone bag. Among the tested configurations, the perovskite conglomerate retained within a silicone bag proved the most effective, achieving a 91% CBZ removal efficiency at a natural pH (6.5). Moreover, the reusability of microparticles was confirmed for three consecutive cycles (Figure 1), as well as through the characterization study using FTIR, Raman, XRD, ICP-OES and SEM-EDS, without important modifications in the material after use. Results confirmed the technology's potential for removing CBZ operating with real conditions. Thus, the proposed process represents an alternative treatment to remove CBZ efficiently in a wide range of concentrations from real wastewater in a continuous treatment with a reasonable energy cost (ca. 27 kW/h·gCZP).

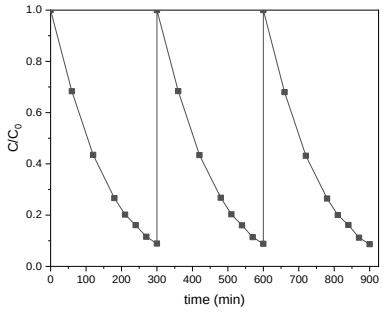

Figure 1: Degradation profiles of CBZ by TDEF in three consecutives uses with ultrapure water matrix. Conditions: [CBZ] = 10 mg/L, aireation = 0.3 L/min, agitation = 300 rpm, intensity = 0.3 A, natural pH (6.5).

Acknowledgements
This work was supported by projects REQUIMTE/LAQV—UIDB/50006/2020, UIDP/50006/2020, LA/P/0008/2020 and EXPL/BII-BIO/0436/2021 and financed by FCT/Ministério da Ciência, Tecnologia e Ensino Superior (MCTES) through national funds. This work was also supported through the Biodiversa & Water JPI joint call for research proposals under the BiodivRestore ERA-Net COFUND program, BiodivRestore-406DivRestore/0002/2020, and cofunding by FCT, Portugal and Project PCI2022-132941 cofunding by MCIN/AEI/10.13039/501100011033. The authors also wish to thank the program supported by Rey Juan Carlos University (URJC) for postdoctoral international stays of young researchers as well as ELECTROCHAR and SLUD4MAT&WATER (PID2021-122883OB-I00) projects financed by URJC and Ministry of Science and Innovation, respectively. A. Puga acknowledges FCT for the Ph.D. grant (2021.08888.BD).

P19

Ring-closing metathesis and heck reactions in the synthesis of isatin-based macrocycles for treating alzheimer's disease

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Scientific topic: Medicinal and pharmaceutical applications

Some of the targets involved in Alzheimer's disease are considered undruggable, which means that these biomolecules do not respond to conventional small molecules.[1] This is the reason why larger molecules began to be considered as potential therapeutics for these targets. Macrocycles for a long time have a privileged status for the treatment of various disease, particularly cancer (Dolastatin, Laulimalide A, Peloruside), anti-microbial (Erythronolide B) and immunosuppressants (Rapamycin, FK-506), showing favorable pharmacological properties.

Our interest has been the development of novel oxindole based macrocycles – which show a large spectrum of biological activities – against neurodegenerative diseases, in particular Alzheimer's.[2,3]

In this communication, we report our efforts on developing novel macrocyclic structures based on isatin and the application of powerful catalytic tools to achieve this objective, using various methodologies that include cross-coupling reactions (e.g. Mizoroki-Heck) and Ring-Closing Metathesis (RCM) approaches (Figure 1).

Furthermore, these compounds will then be screened *in vitro* against β-secretase (BACE-1), responsible for β-amyloid formation in Alzheimer's disease.

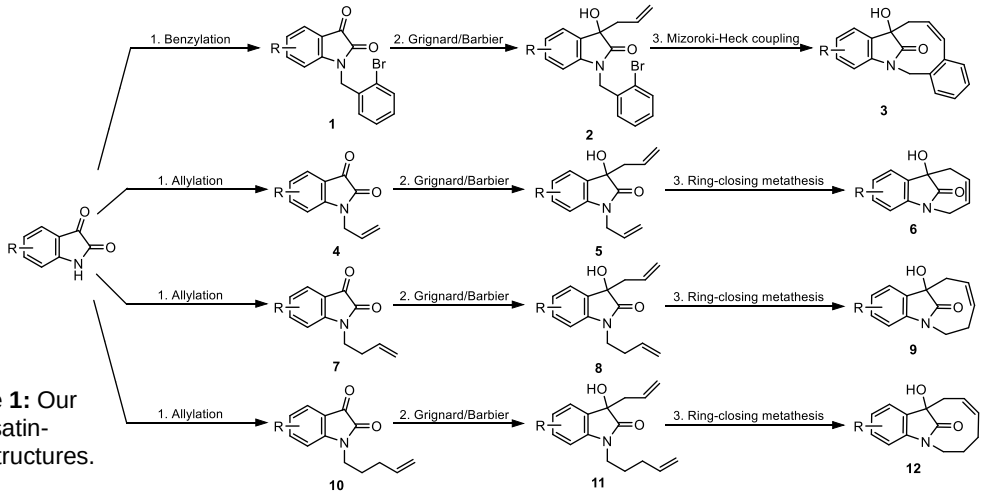

Figure 1: Our synthetic approach to isatin-macrocyclic structures.

Acknowledgements
We thank to the FCT for funding through the strategic project UIDB/00313/2020 | UIDP/00313/2020 to Coimbra Chemistry Centre – Institute of Molecular Sciences (CQC-IMS).

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P20

Estrogen removal through adsorption on carbon materials prepared from biomass wastes: A review

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Scientific topic: Porous materials for energy and environment

Due to the rapid urbanization and industrialization of our world, inadequate waste disposal into land and aqueous matrices has been a deepening environmental and health concern. Substances such as pharmaceuticals, heavy metals, pesticides, surfactants, and petroleum derivatives can be classified as emerging pollutants, thanks to their ever-growing presence and accumulation in the biosphere, especially in water bodies and even in our domestic drinking water[1]. Many of these emerging pollutants can also be classified as micropollutants, since they can harm living beings in very low concentrations, in the magnitude of micrograms per liter (µg/L) or nanograms per liter (ng/L)[2]. An especially worrying class of micropollutants are endocrine disruptors, which are compounds that act directly and deregulate the endocrine system in both humans and animals. Endocrine disruptors can consist of natural hormones, such as estrone (estrogen E1), 17β-estradiol (estrogen E2), and estriol (estrogen E3), or synthetic, such as 17α-ethinylestradiol (estrogen EE2), that owing to their nature as micropollutants, are not easily removed by conventional treatment processes in water and sewage treatment plants, leading to them becoming dangerous emerging pollutants[3]. In this work, a bibliographic review was carried out regarding adsorption studies aiming the removal of estrogens through biomass-based adsorbent materials. The review focused mainly on the selection of several features namely: the type of adsorbate and adsorbent, activation method, adsorption capacity, equilibrium, and kinetic mechanisms. Hence, selected relevant literature studies are summarized in Table 1.

Table 1: Selected adsorption studies from literature and the respective main results

Estrogens	Adsorbent	Activation	Adsorption capacity (mg/g)	Isotherm Model	Kinetic Model	Ref.
E1, E2	Banana peal	No activation	0.387 – 0.420	Freundlich	PSO	4
EE2	Palm kernel shell	Carbonization	1.68	Langmuir	General	5
E1, E2, E3	Walnut shell	Pyrolysis	0.80 – 2.80	Freundlich	PSO	6
E2	Corn straw	Pyrolysis	99.8	Langmuir	PSO	7
E2	Wood sawdust	K_2FeO_4 + pyrolysis	99.67 – 133.45	Langmuir	PSO	8

Table 1 presents a few selected studies from a wide variety of works related to this topic published in recent years, with wood sawdust activated by potassium ferrate and pyrolysis showing the best adsorption capacities.

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P21

Continuous flow sequential catalytic processes for scalable production of eugenol derivatives

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Scientific topic: Other application(s)

Eugenol (4-allyl-2-methoxyphenol) is a naturally occurring molecule with well-documented antioxidant, anti-inflammatory and antimicrobial properties. Eugenol derivatives are also widely used as a flavoring agent in foods, as well as in fragrance and cosmetic industries.[1] In this regard, there has been an increasing interest in the implementation of multi-catalytic sequential reactions for transformation of eugenol into varied products, which may lead to intensified olfactory characteristics and enhanced properties, resultant of the presence of different chemical moieties.[2] In particular, due to the need of the fragrance industry to implement safer operation conditions and decrease costs, continuous-flow systems have been developed in the last years,[3] providing several advantages when compared to traditional discontinuous processes, namely the unique control over reaction parameters (such as temperature and pressure) and a more efficient mass transfer.[4]
In this communication, we present our recent studies regarding the development of catalytic multi-step processes under continuous-flow conditions, to transform eugenol into new potential fragrances, Figure 1.[5] Two approaches are described: i) catalytic epoxidation followed by CO_2 cycloaddition to obtain the correspondent cyclic carbonate (with up to 7.7 g product/day); and ii) a catalytic hydroformylation/acetalization sequential process, which operates through a multi-stage flow system consisting of a tubular reactor for the Rh-catalyzed hydroformylation, coupled in series with a K10 packed bed reactor for the aldehyde acetalization step (with up to 10.0 g of product/day).

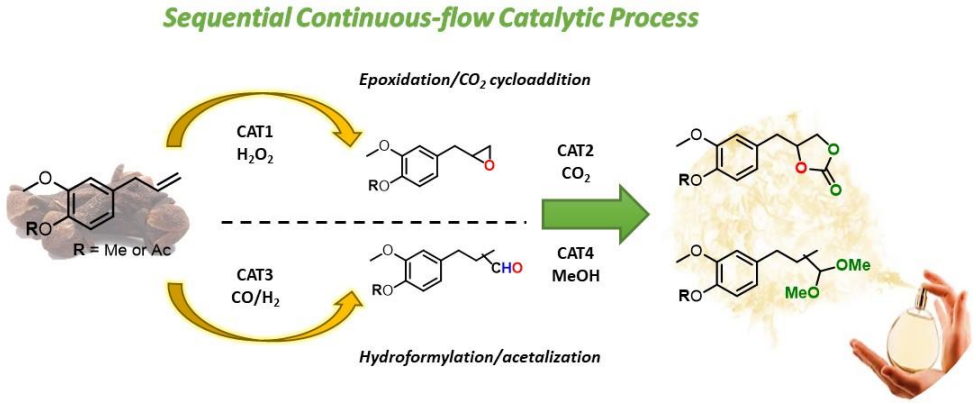

Figure 1: Production of eugenol derivatives through continuous flow sequential catalytic processes.

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P22

Synthesis of Hierarchical Zeolites by Template-Assisted Desilication Hydrothermal Method for Electrocatalytic Applications

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Scientific topic: Heterogeneous catalysis

Zeolites are well-known for their utility as catalysts and or supports for metal-based catalysts, owing to their expansive surface area and robust mechanical and chemical stability, which prevent leaching of the metal phase. However, the presence of micropores imposes constraints on the diffusivity of reactants and products. Addressing this challenge, the secondary mesoporous network inherent in hierarchical zeolites emerges as a promising solution. This distinct texture enhances mass transfer phenomena within the pores, thereby promoting improved accessibility to the active sites.[1] In this work, NaY zeolite was modified by acid wash followed by hydrothermal (150 °C) desilication with NaOH in the presence of CTAB for different treatment times. Bimetallic zeolites were prepared from conventional and hierarchical zeolites by ion-exchange. N_2 physisorption, X-Ray Diffraction (XRD), and Transmission Electron Microscopy (TEM) were used for characterizing all the materials. Bimetallic zeolite-modified electrodes based on Carbon Toray were investigated in aqueous media, at different pH, for the electrochemical oxidation of glycerol. A by-product of biodiesel production, glycerol is a raw material for synthesizing various valuable chemicals. Its oxidation is particularly interesting owing to the presence of three distinct alcoholic functions, which allows for the generation of a diverse array of oxidized products (Figure 1).[2] Several studies reported that electrodes modified with metal-containing zeolites exhibit excellent mechanical and chemical stability, with leaching of the metal phase not observed.[3] The structural differences between the conventional and hierarchical zeolites promote a different catalytic behaviour in the electrolyses of glycerol oxidation.

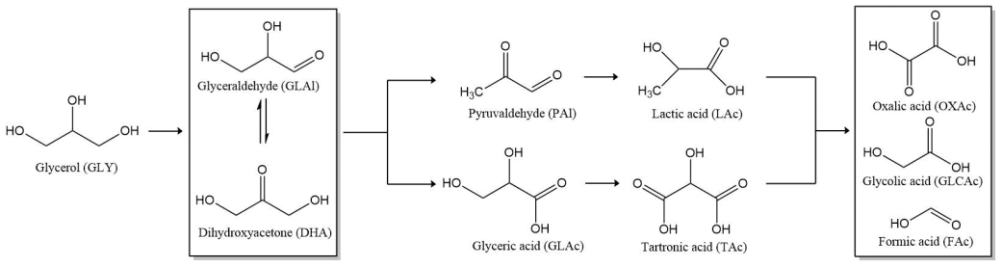

Figure 1: Simplified scheme for glycerol oxidation [2].

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