GFZ 2026

41ème réunion annuelle

30 mars - 2 avril

Village Vacances **Port-Bail**, Normandie, France

Groupe Français des Zéolithes

GFZ 2026

41ème réunion annuelle

Lundi 30 mars

- 14:30 Navette depuis la gare de Valognes
- 15:15 Accueil des participants à la réunion annuelle GFZ et installation des posters
- 16:30 Cérémonie d'ouverture
- 16:45 Plénière - D. Serrano
- 17:30 Session Flash
- 18:00 Session Exposants
- 19:30 Apéritif de bienvenue
- 20:00 Dîner

Mardi 31 mars

- 09:15 Keynote - V. Zholobenko
- 09:45 O1.1. B. Yeskendir
- O1.2. T. Spanjersberg
- O1.3 N. Martin
- 10:30 *Pause*
- 11:00 O1.4. L. Orban
- O1.5. I. Ermakov
- O1.6. J. Prech
- O1.7 H. Al Assaad
- 12:15 *Déjeuner*
- 13:45 Keynote - F. Pourpoint
- 14:15 Session Flash
- 14:45 *Pause*
- 15:00 Session Poster
- 16:15
- 17:00 Apéritif - Manoir
- 19:30
- 20:00 Dîner

Mercredi 1 avril

- 09:00 Plénière - B. Louis
- 09:45 O3.1. L. Pinard
- O3.2. M. Bectoras
- O3.3. K. Bernardo-Gusmao
- 10:30 *Pause*
- 11:00 O3.4. M. Bonneau
- O3.5. P. Dabrowski
- O3.6. M. Qassab
- O3.7. A. Vicente
- 12:15 *Déjeuner*
- 13:45 Plénière - G. Maurin
- 14:30 O2.1. E-B. Zerifi
- O2.2. M. Vidal
- O2.3 J. Duplessis-Kergomard
- 15:15 *Pause*
- 15:30 Session Poster
- 16:30
- 17:00 O2.4 L. Benariac-Doumal
- O2.5. P. Al Azzi
- O2.6 M. Mazur
- O2.7 B. Claessens
- 18:30 Apéritif surprise (sponsorisé Anton Paar)
- 20:00 Banquet
Animation surprise
(sponsorisé Anton Paar)
- 22:00 Soirée Karaoké

Jeudi 2 avril

- 09:00 Keynote - K. Larmier
- 09:30 Keynote - Prix Jeune Chercheur.se
- 09:50
- 10:00 Assemblée Générale & Remise des prix
- 11:45 Navette pour Valognes

Groupe Français des Zéolithes

GFZ 2026

41ème réunion annuelle

Programme Scientifique

Lundi 30 mars 2026

15:15 Accueil des participants et installation des posters

16:30 Cérémonie d'ouverture

Chair : Emily Bloch & Eddy Dib

16:45 **Plénière : David Serrano** “Synthesis of dendritic MFI zeolites“

17:30 **Présentations Flash**

P1-1 **I. Hassan** “Synthesis of NMC MOFs from spent lithium ion battery cathodes: Comparison of Sonochemical and Mechanochemical routes“

P1-2 **M. Mezni** “Synthesis of Zeolites from natural clay: Study of synthesis parameters”

P1-3 **H. El Bouhamydy** “Mixed Valence HKUST-1 As an Heterogenous Catalyst for Click Reaction (CuAAC): A Comparative Study“

P1-4 **S. Feyzaieyva** “A mixed-ligand strategy to enhance MOF stability and functionality: Case study on copper MOFs and CO_2 adsorption”

P2.1 **J. Han** “Targeted Modification of ZSM-5 for High-Efficiency Co-Production of Para-Xylene and Light Olefins from Methanol–Toluene Co-Conversion”

P2.2 **N. Chaouati** “Additive and Synergistic Effects in USY/ZSM-5 Systems: Role of Acidity, Composition, and Phase Intimacy in n-Hexane Cracking“

Programme Scientifique

Lundi 30 mars 2026

18:00 **Présentations Exposants**

EXH-1 Présentation de la société **Anton Paar**, par Troyaux Rihab, Zakhia Douaihy Rita

EXH-2 Présentation de la société **Micromeritics**, par Castelain Hélène, Alexandre Moury, Kahina Moussi

EXH-3 Présentation de la société **Surface Measurement Systems**, par Hanif Aamir, Mcintyre Sean, Nagazi Yassine

EXH-4 Présentation de la société **MICROTRAC Verder**, par Amoury Bilal

EXH-5 Présentation de la société **Equilabo**, par Stachowiak Christian

18:30 Quartier libre

19:30 Apéritif de Bienvenue

20:00 Dîner

Groupe Français des Zéolithes GFZ

GFZ 2026

41$^{\text{ème}}$ réunion annuelle

Programme Scientifique

Mardi 31 mars 2026

Chair : Louwanda Lakiss & Andrey Ryzhikov

09:15 **Keynote : Vladimir Zholobenko** "Characterisation of active sites and adsorbed species in zeolites"

09:45 **Oraux Thème 1- Synthèse et mise en forme**

O1-1 **B. Yeskendir** "3D-printed geopolymers supporting MFI-type zeolite for glucose isomerization"

O1-2 **T. Spanjersberg** "Lifespan enhancement through defect formation in ZSM-5 zeolites"

O1-3 **N. Martin** "Phase-selective high pressure hydrothermal synthesis of zeolites from kaolinite"

Pause

11:00

O1.4 **L. Orban** "Synthesis of dendritic Sn-MFI zeolites"

O1.5 **I. Ermakov** "Steam-assisted crystallization of Sn-BEA zeolite and its catalytic performance in reactions of cyclohexanone conversion"

O1.6 **J. Přech** "Zeolite carrier hydrophilicity in Pd/zeolite catalysts has to match with substrate polarity in alkyne semihydrogenation"

O1.7 **H. Al Assaad** "Photochemical Design of MOF@Polymer Hybrid Architectures for Advanced Mixed Matrix Membranes"

12:15 *Déjeuner*

Programme Scientifique

Mardi 31 mars 2026

Chair : Bogdan Harbuzaru & Alexandre Legrand

13:45 **Keynote : Frédérique Pourpoint** "Understanding the structural changes in MOFs using high-field NMR"

14:15 **Présentations Flash**

P2.3 **M. Benamar** "Hierarchical MOR Zeolites: Unravelling Microporosity Evolution through Organic Probe Adsorption"

P2.4 **A. Hanif** "Influence of Water, NO_2, and SO_2 on CO_2 Adsorption Performance of Zeolite 13X Under Post-Combustion Conditions"

P3.1 **N. Martin** "A multi-technique investigation of organochlorine adsorption in zeolites: linking calorimetry, TG-MS and DFT approaches"

P3.2 **J. Al Atrach** "Direct air capture of CO_2 by Ba-exchanged GIS-type zeolite"

P3.3 **H. Piva Diogenes** "Silanol Removal Enhances VOC Adsorption in Mo-MFI Zeolites: An Experimental–Computational Approach"

P3.4 **K. Borba** "Chemical Recycling of PET for MOF Synthesis"

Pause

15:00 **Session Poster**

17:00 Apéritif au manoir

20:00 Dîner

Groupe Français des Zéolithes

GFZ 2026

41ème réunion annuelle

Programme Scientifique

Mercredi 1er avril 2026

Chair : Emily Bloch & Alexandre Legrand

09:00 **Plénière : Benoît Louis** "Zeolites as Game Changers for the XXIth Century Energy Roadmap ?"

09:45 **Oraux Thème 3 - Applications (environnement, énergie, santé)**

O3-1 **L. Pinard** "Développement d'un nouveau protocole de spectrométrie de masse en temps réel dédié à l'optimisation rapide de la pyrolyse catalytique de la biomasse"

O3-2 **M. Bectoras** "Encapsulated iron oxide nanoparticles within the intrawall pores of SBA-15 via melt infiltration as efficient Fenton-like catalyst for lindane degradation"

O3-3 **K. Bernardo-Gusmao** "Exploring Dendritic Zeolites as Catalytic Supports for Ethylene Oligomerization"

Pause

Chair : Carmen Ciotonea & Eddy Dib

11:00

O3.4 **M. Bonneau** "MIL-160: A Sustainable Adsorbent for Water Harvesting and Adsorption Cooling Technologies"

O3.5 **P. Dabrowski** "Impact du Cérium sur l'adsorption de diiode gazeux et sa conversion dans des Metal-Organic Frameworks de type UiO-66"

O3.6 **M. Qassab** "Plastic Pyrolysis over Extra-Large Pore Zeolites"

O3.7 **A. Vicente** "Real time tracking of Gallium oxides in MFI zeolites during reaction by operando approaches"

12:15 *Déjeuner*

Groupe Français des Zéolithes

GFZ 2026

41ème réunion annuelle

Programme Scientifique

Mercredi 1er avril 2026

Chair : Emily Bloch & Benoît Louis

13:45 **Plénière : Guillaume Maurin** "Computation-guided Advances in MOFs"

14:30 **Oraux Thème 2 - Caractérisation et modélisation**

O2-1 **E-B. Zerifi** "Cation-Exchanged Ferrierite Zeolite as a Promising Adsorbent for Radon: A Combined Computational and Experimental Study"

O2-2 **M. Vidal** "Insights into fe-oxidant interactions (N_2O, O_2, CO_2) within FER zeolite frameworks"

O2-3 **J. Duplessis-Kergomard** "Putting ZIF-8 in Shape: ZIF-8 / Polymer Extrudates for Gas Phase Alcohol/Water Separations"

Pause

15:30 **Session Poster**

Chair : Eddy Dib & Bogdan Harbuzaru

17:00

O2.4 **L. Benariac-Doumal** "Neutron diffraction for the localization of coke in zeolite catalysts during methanol-to-hydrocarbons conversion"

O2.5 **P. Al Azzi** "From Equilibrium to Dynamics: Benchmarking the CO_2 Capture Performance of ZMQ-1"

O2.6 **M. Mazur** "In-situ heating electron microscopy of metal species in 2D zeolites: tracking metal–support interactions and thermal stability of zeolite-supported catalysts"

O2.7 **B. Claessens** "How does structured adsorbent channel heterogeneity influence the efficiency of adsorptive CO_2 capture?"

18:30 *Apéritif surprise (sponsorisé par Anton Paar)*

20:00 *Banquet & Animation surprise (sponsorisé Anton Paar)*

22:00 *Soirée Karaoké*

Programme Scientifique

Jeudi 2 avril 2026

Chair : Emily Bloch & Louwanda Lakiss

09:00 **Keynote : Kim Larmier** “Zeolitic catalysts for the conversion of biomass-based sugars into platform chemicals”

09:30 **Keynote : Prix Jeune Chercheur/Chercheuse 2026**

Pause

10:00 Assemblée Générale & Remise des prix

11:45 Navette pour Valognes

Plénières

Synthesis of dendritic MFI zeolites

David P. Serrano[a,b]

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[b]*Chemical and Environmental Engineering Group, URJC, 28933, Móstoles, Madrid, Spain.*

Dendritic nanomaterials possess radially oriented meso-macropores with a high degree of connectivity, which provides them with very accessible 3D disordered superstructures.[1] These materials have been explored recently as supports of a number of guest molecules and functionalities, leading to an increasing number of studies in a variety of fields: catalysis, pollutant decontamination, energy harvesting and storage, sensors, CO_2 capture and biomedical applications.[2,3]

In contrast, the synthesis of zeolitic materials with dendritic nano-architectures has been revealed rather elusive probably because zeolites possess rigid crystalline structures in comparison with amorphous silica. However, as reported in recent works,[4,5] our research group has been successful in the synthesis of dendritic MFI zeolites by the combination of two strategies that were earlier individually applied for the preparation of hierarchical (non-dendritic) zeolites: i) crystallization of functionalized protozeolitic nanounits and the use of amphiphilic organosilanes.

Following this approach, ZSM-5 materials with a well-defined and fully crystalline dendritic nano-architecture have been developed, showing outstanding accessibility, enhanced textural properties (with a multi-modal porosity, external surface areas over 300 m^2/g and total pore volumes up to 1 cm^3/g) and a balanced Bronsted/Lewis acidity.

These materials have shown so far to present remarkable properties as catalysts in a variety of reactions, such as limonene and terpenes epoxides isomerization,[6,7] aldol-condensation synthesis of jet fuel precursors,[8] polyolefin cracking[4] and hydrogen production by methane decomposition.[9] Varying the synthesis conditions, it has been possible to obtain dendritic MFI materials with diverse morphologies (Figure 1) and controllable textural and acidic properties. Likewise, replacement of Al by other framework heteroatoms (Ga, Fe, B, Ti and Sn) has been accomplished while keeping the dendritic features, which opens huge opportunities for their application in a great variety of sectors.

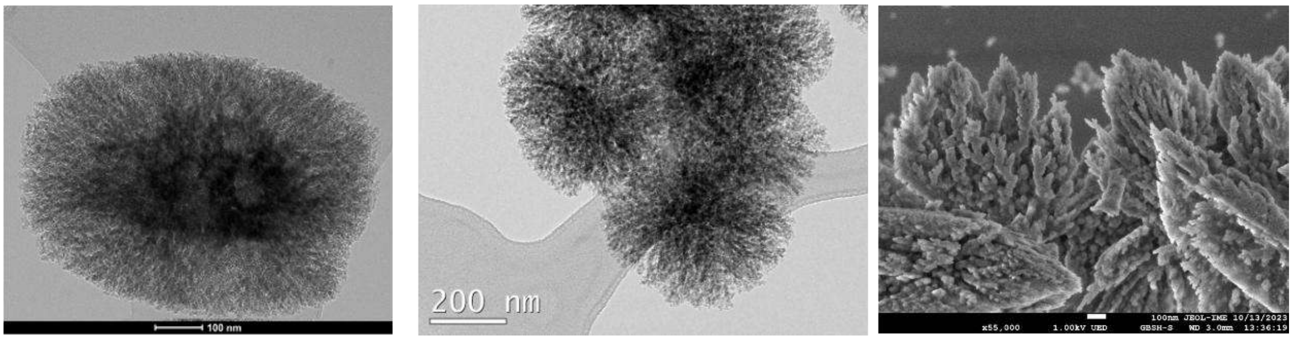

Figure 1. TEM/SEM images of dendritic ZSM-5 zeolites showing different nano-architectures: core-shell (left), stars (centre) and tree-like (right).

References:
[1] A. Maity and V. Polshettiwar, *ChemSusChem,* **2017**, *10*, 3866–3913.
[2] P. Hao et al. *Nanoscale Advances,* **2020**, *2*, 1792–1810.
[3] Y. Wang et al. *Journal of Materials Chemistry A,* **2019**, *7*, 5111–5152.
[4] M. Alonso-Doncel et al. *Journal of Energy Chemistry*, **2023**, 80, 77–88.
[5] M. Alonso-Doncel et al. *Crystal Growth & Design*, **2023**, 23, 5658-5670.
[6] L.A. Gallego-Villada et al. *Chemical Engineering Journal*, **2024**, 498, 155377.
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[8] D. de la Calle et al. *Fuel*, **2026**, 412, 138137.
[9] B.P. Nicola et al. *Microporous and Mesoporous Materials*, **2026**, 401, 113939.

THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Computation-guided Advances in MOFs

Guillaume Maurin
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MOFs offer unparalleled structural tunability for energy and environmental applications. Yet, their vast chemical and structural diversity make exhaustive experimental screening unfeasible. Computational modelling, empowered by machine-learning (ML) methods now provides a powerful route to accelerate discovery and optimization.

Our recent work shows how Machine Learning Potentials (MLPs) bridge quantum accuracy and large-scale efficiency, enabling predictive modelling of flexible frameworks that undergo structural transitions under external stimuli. In particular, MLPs capture strong host–guest interactions in MOFs with open metal sites, inaccessible to traditional force fields, allowing accurate predictions of adsorption and mechanical behaviour.

We also explore mixed-matrix membranes (MMMs) combining MOFs with polymers for gas separation. Through multiscale simulations, we reveal how polymer rigidity and MOF surface chemistry control interfacial pore structure and, consequently, gas transport. Importantly, we show that pore shape, beyond size, governs molecular selectivity.

Together, these computational advances establish a rational design framework for next-generation MOFs and hybrid membranes, bridging atomistic insight with real-world performance.

THEME X Theme 1 : Applications for the environment, energy, and health

Zeolites as Game Changers for the XXIth Century Energy Roadmap ?

Benoît Louis
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"Super big-two" zeolites, having either the FAU or MFI topology, are by far the most important active catalysts used in refineries, as for instance in the fluid catalytic cracking (FCC) process for converting gasoil into valuable products [1].

Unfortunately, with growing fossil fuel utilization and industrial activities, along with World population increase to 8 billion, the amount of greenhouse CO_2 emissions is continuously rising, leading to severe climate change issues [2]. A new paradigm needs therefore to be set with the emergence of alternative energy sources or at least an energy mix.

In the energy context of the XXth century, after decades of significant optimization of zeolite synthesis and properties, along with the development of sophisticated characterization tools and modelling, those amazing microporous materials became the leaders for performing acid-catalyzed reactions.

The question now arise, will zeolites and emerging microporous materials still act as leaders in the new energy roadmap of the XXIth century? In the extended presentation, we will try to answer this question while selecting few issues that we are currently facing and (hopefully) solve: CO_2 capture and utilization, methanol economy [3], or viable production of biofuels.

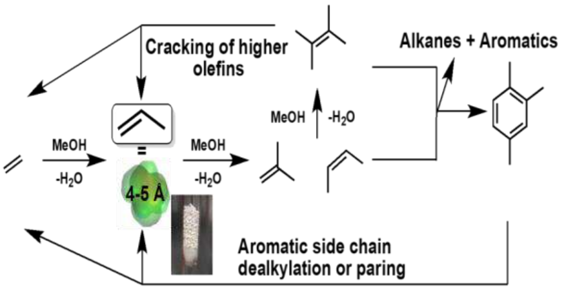

Fig. 1. Methanol conversion into hydrocarbons over shaped ZSM-5 zeolites

Selected applications (as in Figure 1) will be presented keeping in mind that one still has to bridge the gap between the lab curiosity and its further scale-up for future industrial implementation: while overcoming issues related to shaping, mass transfer and economics.

References

[1] V. Blay, B. Louis, R. Miravalles, T. Yokoi, K.A. Peccatiello, M. Clough, B. Yilmaz, ACS Catalysis 7 (2017) 6542-6566.
[2] W. Gao, S. Liang, R. Wang, Q. Jiang, Y. Zhang, Q. Zheng, B. Xie, C.Y. Toe, X. Zhu, J. Wang, L. Huang, Y. Gao, Z. Wang, C. Jo, Q. Wang, L. Wang, Y. Liu, B. Louis, J. Scott, A.C. Roger, R. Amal, H. Heh, S.E. Park, Chem. Soc. Rev. 49 (2020) 8584–8686.
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Keynotes

THEME

☐ Theme 1 : Applications for the environment, energy, and health

X Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

Understanding the structural changes in MOFs using high-field NMR

A. Nadol,[a] F. Venel,[a] R. Giovine,[a] O. Lafon,[a] C. Volkringer,[a] **F. Pourpoint**,[a,b]

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[b] *Institut Universitaire de France, IUF, 1 rue Descartes, 75231 Paris Cedex 05, France*

Metal-Organic Frameworks (MOFs) are widely recognized for their versatile applications, such as catalysis, sensing, gas adsorption, membranes technologies, etc. These applications inherently involve exposure to external stimuli. Enhancing MOF performance therefore requires a thorough understanding of stimulus-induced structural modifications, including the formation of defects. Solid-state Nuclear Magnetic Resonance (ssNMR) spectroscopy is a powerful atomic-scale technique that enables detailed investigation of local structure, dynamics and presence of defects.

We focused on the stability of the MOFs in presence of water. In particular, quadrupolar nuclei such as ^{17}O[1] or ^{91}Zr[2] with I = 5/2, provide unique insight into the atomic-level structural modifications of inorganic cluster in Zr-based UiO-66. Although the observation of these insensitive isotopes represents a significant experimental challenge, we demonstrate strategies to overcome these limitations and extract valuable structural information.

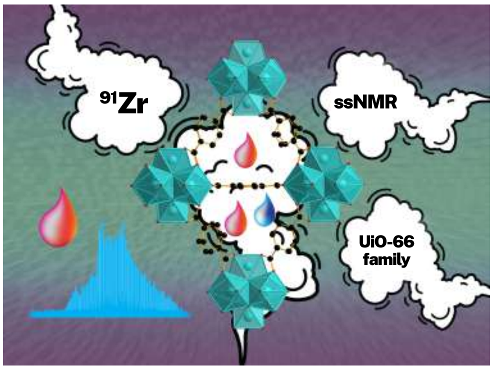

Fig. 1. ^{91}Zr NMR helps to characterize the structural modifications of the cluster in Zr-based MOF in presence of steam at different temperatures.

References

[1] F. Venel, R. Giovine, D. Laurencin, J. Špačková, S. Mittelette, T.-X. Métro, C. Volkringer, O. Lafon, F. Pourpoint, *Chem. Eur. J.* **2024**. DOI: 10.1002/chem202302731.
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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Characterisation of active sites and adsorbed species in zeolites

Vladimir Zholobenko [1,2]
1 School of Chemical and Physical Sciences, Keele University, United Kingdom
2 Department of Chemistry, Moscow State University, Moscow, Russian Federation

Zeolites are essential for a host of major industrial processes, and studies into zeolite science have increased dramatically over recent decades, reflecting the growing understanding and application of these versatile materials. Millions of tons of crude oil are daily converted on zeolite-based catalysts in oil refining and petrochemical industries for the production of petrol and diesel, ethylene, propylene and simple aromatics for the production of polymers, plastics, etc. These global industries make use of the interactions between the hydrocarbons and the catalyst active sites. Detailed understanding and modelling of these processes is based on the knowledge of the fundamental parameters of the interaction between the zeolite and substrates as well as their concentrations during adsorption, diffusion and chemical transformations, which can be monitored using FTIR spectroscopy. However, the quantitative analysis and application of the classic Bouguer-Lambert-Beer law to heterogeneous catalytic systems is challenging, and the accuracy of the reported data can be limited by the equipment available and the methodology utilised in such research.

This work is focused on the quantitative approaches to the characterisation of active sites and adsorbed species in zeolites, especially under in situ and operando conditions. In particular, methodologies combining high-precision thermogravimetry and FTIR spectroscopy, FTIR and solid-state NMR, as well as the application of ultra-fast FTIR spectroscopy are considered.

VZ thanks colleagues from the Laboratoire Catalyse et Spectrochimie (Caen, France), Keele University (UK) and Moscow State University (RF) for their invaluable contribution. Financial support of the Russian Science Foundation (grant №23-73-00005, https://rscf.ru/project/23-73-00005/) and the MSU research programme (No. AAAA-A21-121011990019-4) is gratefully acknowledged.

THEME

☐ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

Zeolitic catalysts for the conversion of biomass-based sugars into platform chemicals

Kim Larmier

IFP Energies nouvelles – Catalysis, Biocatalysis and Separation Division, Etablissement de Lyon, Rond-point de l'échangeur de Solaize - BP 3- 69360 Solaize – France - kim.larmier@ifpen.fr

Zeolites are key catalytic materials for the development of sustainable chemistry and processes that have attracted a lot of attention over the last decades. Herein, we will showcase two examples of the use of zeolitic materials for the production of platform molecules from biomass-based sugars.

First, we will expose a series of work regarding the effect of introducing mesoporosity in H-faujasite catalysts for the conversion of fructose to 5-HydroxyMethylFurfural (5-HMF) (Figure 1a). After detailing the reaction mechanism at stake, structure-activity relationships are explored using chemometric analyses to decipher the effect of the numerous parameters of the zeolites.

We then turn to the use of Lewis acid Sn-beta zeolites for the production of short-chain chemicals, lactic acid in particular, from glucose (Figure 1b). The reaction mechanisms are investigated using a combination of isotopic labelling strategies and molecular modelling (DFT). We provide unprecedented detail at the molecular level regarding the key intermediates and chemoselectivity to explain the experimental observations.

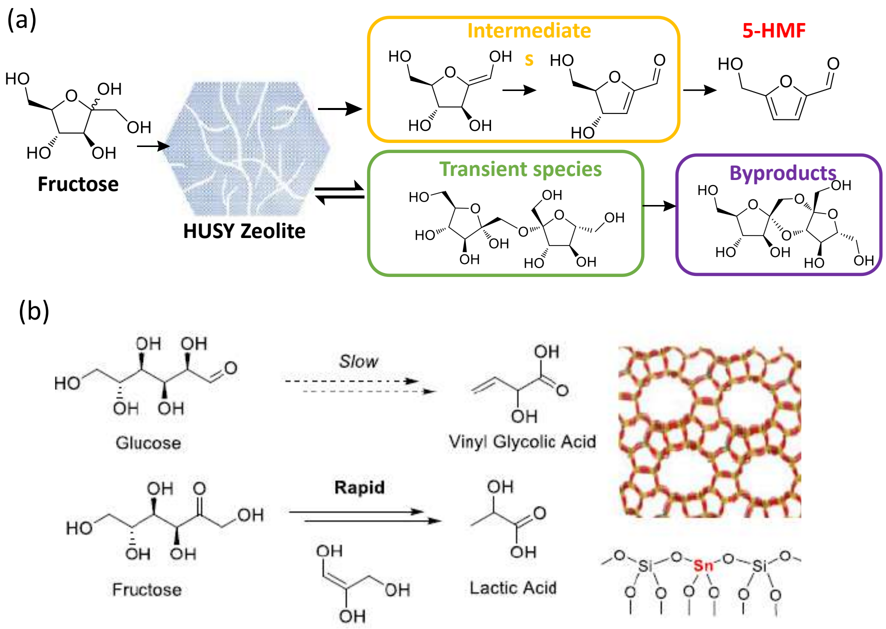

Fig. 1. (a) Mesoporous H-faujasite zeolites for the conversion of fructose to 5-HMF ; (b) Sn-Beta catalysts for the conversion of glucose to lactic acid.

Oraux

Thème 1
Synthèse et Mise en Forme

THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☒ Theme 3 : Synthesis and shaping

3D-printed geopolymers supporting MFI-type zeolite for glucose isomerization

Y. Khadiri,[a] Y. Ettahiri,[b] B. Yeskendir,[a] M. Guessasma,[b] C. Pelegris,[b] J. Dhainaut[a]
[a] *Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France.*
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Thanks to their unique combination of physico-chemical properties, zeolites are widely used catalysts at the industrial scale [1]. Among diverse zeolite types, MFI zeolite shows adjustable acidity and excellent hydrothermal stability, making it a prime choice for biomass valorization [2-3]. However, limited diffusion within the micropores remains a major challenge for conversion of bulky molecules in liquid phase toward further upscaling [4-5].

In this work, a geopolymer (GEO) was used as a stable, low-cost, and environmentally friendly material to shape custom-made monoliths by additive fabrication [6] (Fig. 1 left), serving as supports for the MFI zeolite. Two approaches were investigated: (i) direct synthesis, which consists of immersing the GEO pieces with the reagents required to form MFI under hydrothermal conditions, and (ii) pseudomorphic transformation, involving a controlled increase in the medium's basicity to dissolve a part of the geopolymer, serving as a source of aluminium cations, while the silicon source and structure-directing agents are added.

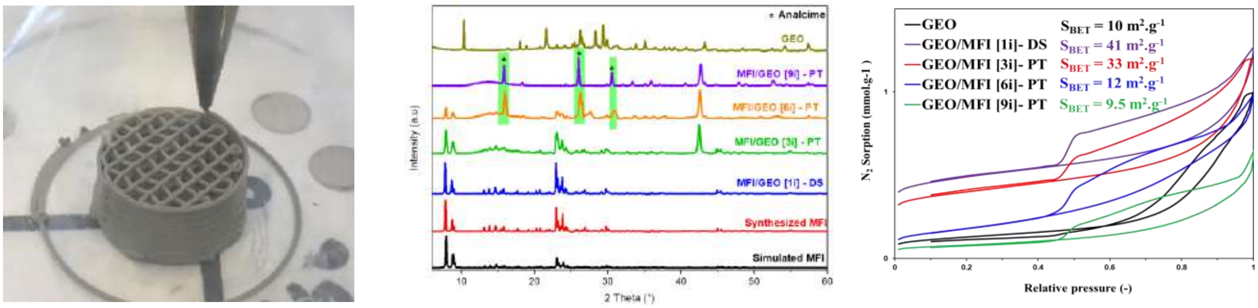

Fig. 1. 3D impression of geopolymer pastes (left), XRD patterns (middle) and N_2 isotherms (right) of the resulted composites.

XRD patterns of such composites show that direct synthesis (DS) and pseudomorphic transformation (PT) at controlled basicity both led to the successful deposition of MFI on the GEO pieces (Fig. 1 middle), while higher basicity promoted the formation of analcime. Moreover, N_2 sorption measurements show that the resulting MFI-based composites exhibit hybrid Type I/II isotherms, reflecting the presence of both zeolite and geopolymer, thus enhancing the concentration of active sites per volume. The solids are under catalytic evaluation for the isomerization of glucose towards fructose.

References

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THEME

☐ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☒ **Theme 3 : Synthesis and shaping**

Lifespan enhancement through defect formation in ZSM-5 zeolites

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Structural defects in zeolites are responsible for significative modifications in their physicochemical properties. Depending on their nature, concentration, and spatial distribution, such defects can either enhance catalytic activity and selectivity or promote rapid catalyst deactivation.[1,2] Therefore, precise knowledge and control of defects are essential for understanding and optimizing the catalytic activity and deactivation of zeolites. Using Formamide (CH_3NO) and Sodium Molybdate (Na_2MoO_4) as additives during the synthesis of ZSM-5, we controlled the type and amount of defects in the ZSM-5 crystals. The properties of the zeolites were characterised by FT-IR, ^{27}Al-NMR, SEM, in situ high-temperature X-ray diffraction, and Ar and N_2 physisorption. In situ XRD was used to follow the phase transition from the monoclinic to orthorhombic space group, elucidating changes in the flexibility and hydration properties of the zeolites (Figure 1).[3,4] This result shows that the additives significantly affected the framework defects. Furthermore, significant reduction in deactivation rate of the ZSM-5 zeolite in the methanol to olefins (MTO) reaction is observed when additives were used (Figure 2). This result highlights the importance of the ability to control defects in zeolites. Strategies utilizing additives during zeolite crystallization opens the avenue towards more stable zeolite catalysts and deeper understanding in the chemistry of defects.

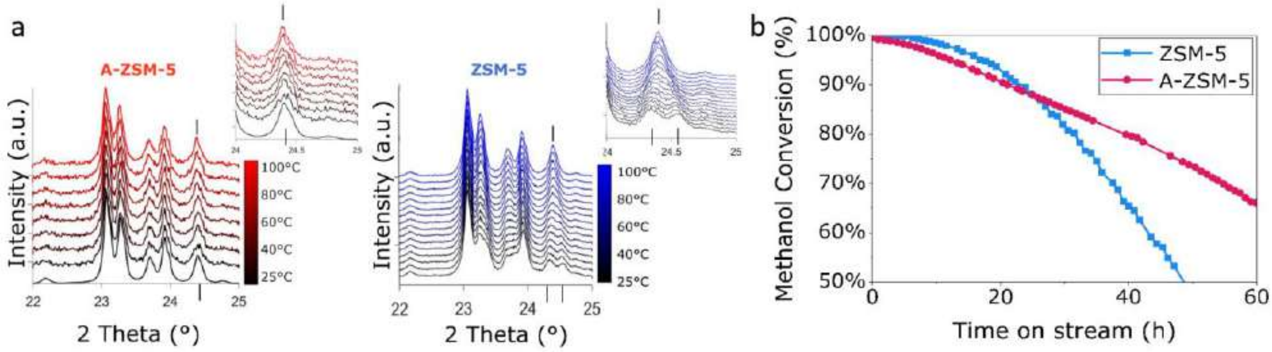

Fig. 1. (a) In situ high-temperature X-ray diffraction of additivated ZSM-5 (A-ZSM-5) and ZSM-5 without additive showing the monoclinic-orthorhombic phase transition for 'ZSM-5'. (b) Methanol-To-Olefin conversion, using A-ZSM-5 and ZSM-5 zeolites, as a function of time on stream.

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☒ Theme 3 : Synthesis and shaping

Phase-selective high pressure hydrothermal synthesis of zeolites from kaolinite

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Zeolites are widely used as catalysts, ion exchangers and adsorbents in many separation processes. The synthesis of zeolites is usually performed following the hydrothermal method by using various chemicals (sources of Si and Al, structure directing agent, etc.). This study presents a phase-selective high-pressure hydrothermal synthesis route for zeolites using natural kaolinite as a sustainable source of silicon and aluminum, with water serving as the solvent under high pressure (100 MPa H_2O pressure) [1]. Kaolinite was first converted into metakaolinite through thermal treatment to obtain an amorphous precursor. Additional silicon sources and sodium hydroxide were introduced to adjust the Si/Al ratio and ensure charge compensation. All reactants were placed in a sealed vessel, and synthesis was carried out under controlled water pressure [2]. The effects of synthesis parameters, including temperature, pressure, and reaction time, on zeolite phase formation and crystal properties were systematically investigated. Faujasite was preferentially formed at relatively low synthesis temperatures, whereas increasing the temperature promoted the crystallization of gismondine and, at higher temperatures, analcime, revealing a clear temperature-dependent phase evolution (Fig. 1a). Furthermore, increasing synthesis pressure led to the formation of larger, well-defined zeolite crystals, while extending the synthesis time resulted in increased specific surface area, indicating improved crystallinity of the obtained zeolite phases.

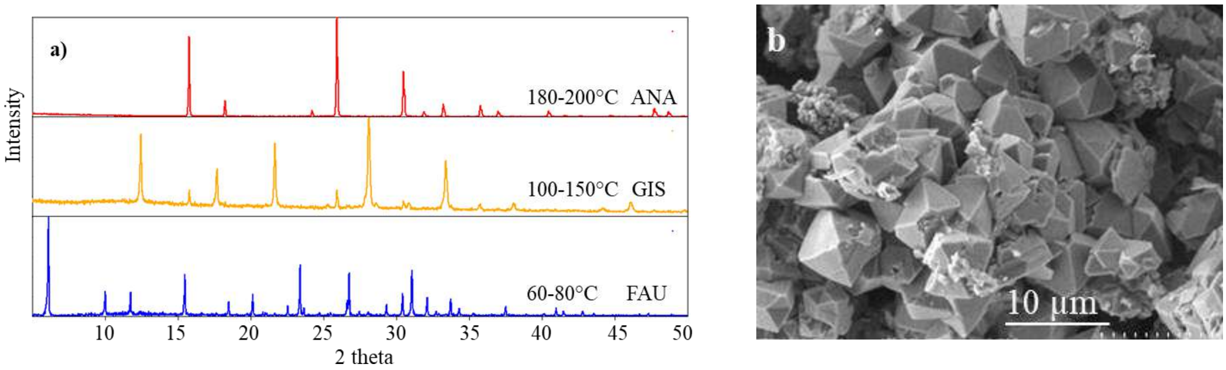

Fig. 1 a). XRD pattern for synthesized zeolites. b). SEM image of synthesized FAU

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THEME

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Synthesis of dendritic Sn-MFI zeolites

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Dendritic ZSM-5 zeolites are distinguished by their singular morphology, defined by the radial orientation of branched crystalline nanounits, their synthesis being recently reported in the presence of an amphiphilic organosilane. [1,2] This dendritic nanoarchitecture leads to a highly interconnected multimodal porosity and enhanced accessibility to the active sites. In this context, the incorporation of tin heteroatoms in the framework of dendritic MFI zeolite samples could produce materials with an interesting combination of Lewis acidity and outstanding textural properties. These new features could also have a deep impact in their catalytic properties. Therefore, the aim of this work has been to investigate the effect of the tin source and its oxidation state in the synthesis of dendritic Sn-MFI zeolites. In addition, the catalytic performance of the resulting samples was evaluated for the production of methyl lactate from dihydroxyacetone, a reaction of relevance in biomass valorization.

In this way, three samples were prepared with different tin sources: tin (II) chloride, tin (IV) chloride and tin (II) ethoxide with a Si/Sn molar ratio of 20 (Samples Sn(II)-MFI-20-Cl, Sn(IV)-MFI-20-Cl and Sn(II)-MFI-20-Et, respectively). From the XRD spectra, it can be inferred that crystalline zeolites were obtained with both tin (II) chloride and ethoxide, while Sn(IV)-MFI-20-Cl sample was partially amorphous, highlighting the importance of the Sn oxidation state in this synthesis. Moreover, the choice of tin (II) ethoxide appeared more convenient than tin (II) chloride as it allows a higher metal incorporation (Si/Sn = 23 instead of 37). In addition, Sn(II)-MFI-20-Et sample exhibits a wide pore size distribution in the mesopore range (Fig. 1b) because of its dendritic morphology (Fig. 1c). Once the optimal tin source was selected, the effect of the Si/Sn ratio was further investigated in terms of textural, morphological, and catalytic properties. The catalytic performance of the resulting materials was then evaluated in the production of methyl lactate (ML) from dihydroxyacetone, alongside pure tin oxides (SnO and SnO_2) and SnO_2 supported on Silicalite-1. All the dendritic Sn-MFI samples exhibited a high methyl lactate yield. In contrast, tin oxides (bulk or supported on Silicalite-1) showed poor performances, clearly demonstrating that the incorporation of tin atoms into the zeolitic framework is essential to generate the specific Lewis acidity required for this reaction.

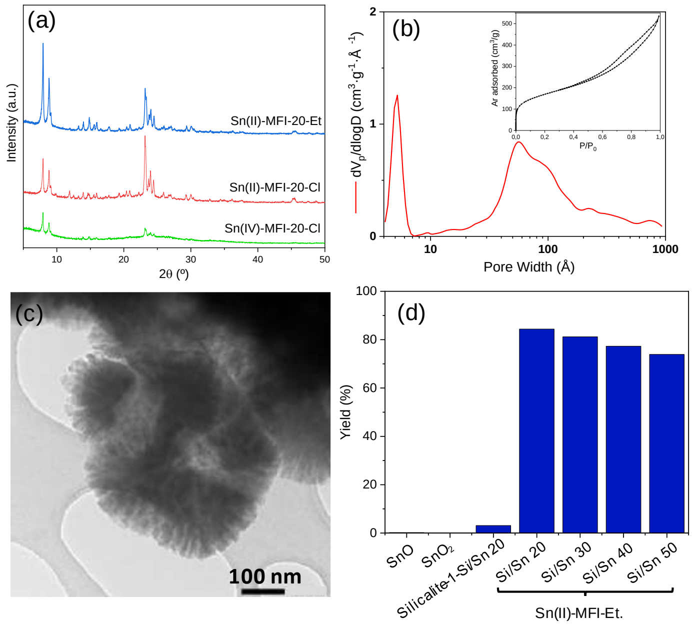

Fig. 1. XRD patterns (a), isotherm (inset) and pore size distribution (Ar 87K) (b), TEM image (c), ML yield (d).

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THEME ☐ Theme 3 : Synthesis and shaping

Steam-assisted crystallization of Sn-BEA zeolite and its catalytic performance in reactions of cyclohexanone conversion

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Sn-containing BEA zeolites are promising catalysts for a wide range of reactions, particularly in biomass valorization, owing to their superior performance compared with zeolites containing other metals that generate Lewis acid sites within the framework. The analysis of the literature indicates that two main approaches are currently employed for the Sn-BEA synthesis: (i) post-synthesis modification and (ii) direct hydrothermal synthesis. The first one is rather easy to accomplish, but it results on materials with large amount of defects and requires the use of corrosive mineral acids. The second one - is often hindered by prolonged crystallization times and significant liquid waste generation. In this context, the aim of this study was to develop novel approach of Sn-BEA zeolite synthesis based on steam-assisted crystallization (SAC) and to investigate its catalytic performance in the Meerwein–Ponndorf–Verley (MPV) and Bayer–Villiger reaction (BV).

The developed steam-assisted conversion (SAC) method utilizes a dry gel precursor, eliminates liquid waste and ensures full autoclave volume utilization, which leads to reduction of energy consumption and simplifies process scale-up. The synthesis was adapted to reduce crystal size by introducing a low-temperature aging step at 100 °C to promote nucleation, successfully decreasing the crystal dimensions from 10 µm to 5 µm. Furthermore, the reaction mixture composition was optimized to maximize tin incorporation into the framework. The optimal Si/Sn ratio was found to be 125; at lower ratios, a BEA/MFI phases are also formed, as confirmed by SEM and XRD analysis.

Kinetic studies of the two-stage synthesis revealed that a phase-pure, highly crystalline Sn-BEA forms within 48 hours—five times faster than conventional hydrothermal synthesis (264 hours). The material obtained exhibits high phase purity, substantial surface area, and a well-developed microporous system. IR spectroscopy of adsorbed pyridine confirmes the presence of both Lewis and Brønsted acid sites, with Lewis acid site concentration comparable to that of hydrothermally synthesized Sn-BEA. The nature of the active sites in Sn-BEA prepared by the SAC method was further probed by ^{119} Sn MAS NMR (DP-CPMG), which confirms the incorporation of tin in different T-position of BEA zeolite.

The Sn-BEA samples obtained were investigated in cyclohexanone conversion to cyclohexanol according to the MPV mechanism and in the oxidation of cyclohexanone to ε-caprolactone with hydrogen peroxide according to the BV mechanism. The conversion of cyclohexanone in the MPV reaction using Sn-BEA was 95% after 10 hours of the reaction and the conversion in the BV reaction using Sn-BEA was 52% after 24 hours of reaction. Thus, the samples synthesized via the developed SAC technique exhibit catalytic characteristics comparable to those of the sample prepared by the conventional hydrothermal method.

In conclusion, the proposed SAC method represents fast and sustainable approach for Sn-BEA zeolites synthesis, achieving catalytic performance comparable to that of hydrothermally synthesized materials. The approach allows for substantial reducion of synthesis time and minimizing waste generation.

Acknowledgements

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
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Zeolite carrier hydrophilicity in Pd/zeolite catalysts has to match with substrate polarity in alkyne semihydrogenation

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Selective hydrogenation of alkynes to alkenes is essential for preparation of polymer-grade olefins and fine chemicals production. Palladium catalysts, particularly the Lindlar catalyst, are the state-of-the-art catalysts allowing preferential hydrogenation of alkynes even in the presence of high excess of corresponding alkene product. However, the Lindlar catalyst has a relatively high content of Pd (5 wt.%), which is partially poisoned with Pb. We recently demonstrated that sub-nanometric Pd species can be stabilized on 2D zeolite carriers increasing the Pd atom efficiency in comparison with the Lindlar catalyst and avoiding use of toxic lead without sacrificing the catalyst selectivity[1]. Here, we investigate in detail the support hydrophilicity, which was found an important parameter influencing selectivity of the resulting Pd/2D zeolite catalysts.

The sub-nanometric Pd clusters (Pd-NC) and Pd nanoparticles (Pd-NP) were formed on layered ZSM-5 carriers by ion-exchange and wet impregnation, respectively, with $[PdCl_2(CH_3CN)_2]$ [1]. TEM imaging showed the Pd clusters had approximately 0.5 nm in diameter without significant dependence on the Si/Al ratio. Pd nanoparticles had 2-10 nm in diameter. Hydrophilicity of the carriers was driven by Si/Al ratio being 15, 30, 60 and pure silica (defect-free pure-silica zeolites are inherently hydrophobic), and it was characterized by water adsorption. Catalytic hydrogenation tests of 1-octyne, 2-methyl-3-butyn-2-ol, and diphenyl acetylene, were carried out in hexane under hydrogen pressure of 5 bar at 25°C. Alkene selectivity in alkyne conversion range 95-99% was used as a key performance indicator.

In pure hydrocarbons, polarity (and thus hydrophilicity) decreases in sequence alkyne>alkene>alkane, unless other polar groups are present (such as aromatic ring or particularly a heteroatom such as -OH group). Accordingly, hydrophilic carrier is beneficial for semihydrogenation of pure hydrocarbons as the alkyne adsorption is preferred over the alkene in the zeolite support close to the Pd phase, which is demonstrated, e.g., by 1-octyne semihydrogenation selectivity over Pd-NP/lam ZSM-5 Si/Al=30 (77%) vs. Pd-NP/pure silica MFI (69%; both at 99% conversion).

Conversely, the hydrophilic Pd-NP/lam ZSM-5 Si/Al=30 provided only 7.8% selectivity at 99% 2-methyl-3-butyn-2-ol conversion, while the hydrophobic Pd-NP/pure silica MFI gave 86% selectivity at the same conditions. The semihydrogenation product 2-methyl-3-buten-2-ol, with a polar -OH group, remains strongly adsorbed on a hydrophilic carrier supporting its over-hydrogenation to 2-methylbutan-2-ol because the alkyne hydrogenation to alkene does not bring a substantial change to the molecule hydrophilicity.

Although, the main selectivity determining parameter is the Pd species size[1], it remains essential to consider substrate polarity and match it with the catalyst carrier hydrophilicity while designing novel, greener, and cheaper alkyne selective hydrogenation catalysts.

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Acknowledgments

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THEME	☒ Theme 1 : Applications for the environment, energy, and health ☐ Theme 2 : Characterization and modeling ☐ Theme 3 : Synthesis and shaping

Photochemical Design of MOF@Polymer Hybrid Architectures for Advanced Mixed Matrix Membranes

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Mixed matrix membranes (MMMs) combine the processability of polymers with the tunable porosity and functionality of inorganic fillers such as metal–organic frameworks (MOFs); however, achieving defect-free architectures with strong filler–polymer interfaces while preserving MOF structural integrity remains challenging. Here, we report a photochemical strategy for the synthesis of UiO-66-based MMMs using a surface-from photopolymerization approach. The method relies on a bifunctional silane-based type I photoinitiator (SPI), developed by our team, which acts as both a surface coupling agent and a radical initiator, enabling polymer growth directly from the MOF surface. SPI-grafted UiO-66 nanoparticles are dispersed in trimethylolpropane triacrylate (TMPTA) and photopolymerized under an inert atmosphere to yield homogeneous, mechanically robust MMMs with tunable filler loadings (Fig. 1A). Photopolymerization in an acetonitrile suspension yields a well-defined core–shell structure with uniformly dispersed fillers, demonstrating the formation of covalent bonds between the polymer matrix and the fillers (Fig. 1B). Structural and morphological analyses confirm efficient SPI grafting and subsequent polymer growth while preserving the crystallinity and morphology of UiO-66 (Fig. 1C, 1D). Real-time FTIR monitoring shows efficient acrylate conversion and identifies an optimal MOF content of 30 wt%, providing the best compromise between high filler incorporation and network formation (Fig. 1E). The strategy is extended to Ag-functionalized UiO-66-$(COOH)_2$, demonstrating its versatility. Silver incorporation maintains the MOF structure and photopolymerization mechanism while imparting strong antibacterial activity against E. coli and S. aureus, enabling interface-controlled MMMs with combined structural integrity and bioactive functionality.

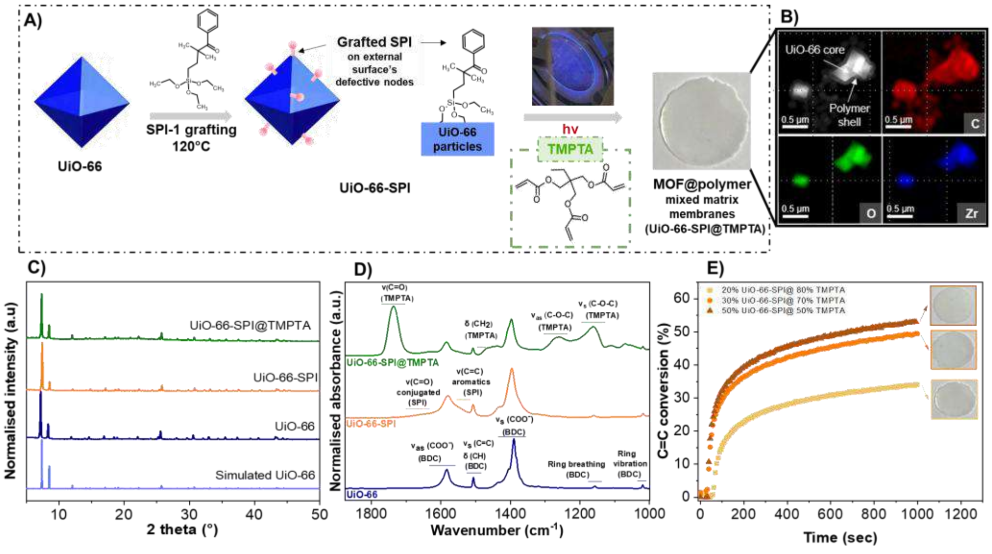

Fig. 1. (A) Photochemical synthesis of MMMs. (B) HAADF-STEM images and EDX elemental maps showing core–shell architecture. (C) PXRD patterns and (D) ATR–FTIR spectra confirming grafting and polymer growth. (E) Photopolymerization kinetics at 365 nm as a function of MOF loading (insets: corresponding membranes).

Oraux

Thème 2
Caractérisation et Modélisation

THEME

☒ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Cation-Exchanged Ferrierite Zeolite as a Promising Adsorbent for Radon: A Combined Computational and Experimental Study

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The sensitivity of low-background detectors used in rare-event physics is often limited by trace radioactive impurities, with radon (^{222}Rn) being one of the most persistent sources. Mitigating this background requires materials capable of selectively trapping radon under ultra-clean conditions. Zeolites have shown an interesting potential for this application [1] and a preliminary Grand Canonical Monte Carlo (GCMC) simulation study predicted as optimal zeolite topology the ferrierite (FER) (Figure 1a), with high charge compensating cations content.

In this study, we have combined molecular simulation techniques in order to predict the Rn adsorption performances and guide the successive experiment. The initial modeling stage allowed us to assess the aluminum distribution along the T-sites of the FER framework and the nature and location of extra-framework cations (Ag^+ , Ni^{2+} , Cu^{2+}). Furthermore, we determined the influence of those parameters on the Rn adsorption performances (Figure 1b). GCMC simulations showed that Ag– and Ni–exchanged FER possess the highest radon adsorption capacity in the low-pressure region, corresponding to the trace partial pressures encountered in low-background detectors. Finally, the FER samples (Si/Al = 10) exchanged accordingly to the simulation outcomes have shown high radon adsorption performances, experimentally corroborating the simulated prediction.

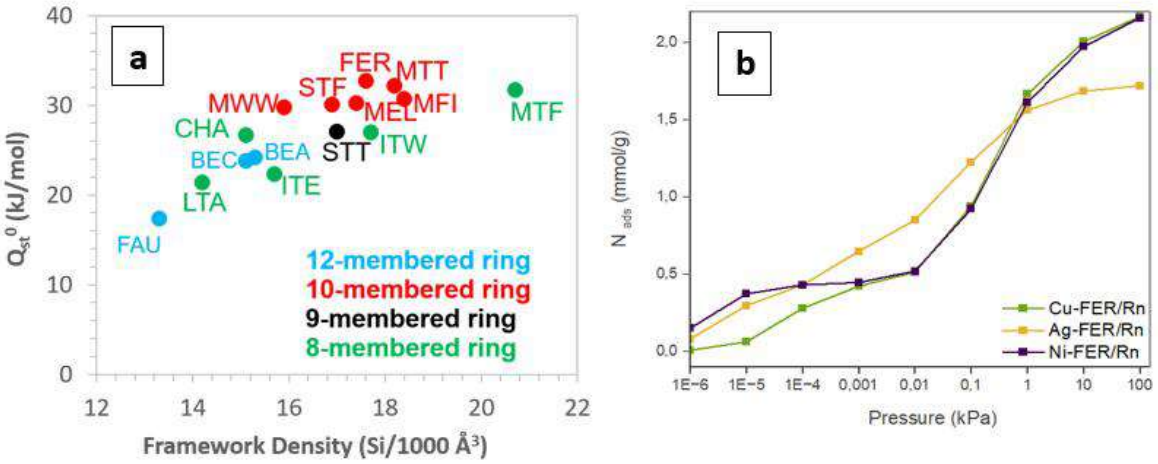

Figure1: Comparative adsorption performance of silica zeolites with varying pore apertures (8-, 10-, 12 MR) **(a)**; Adsorption isotherms of Rn on cation-exchanged FER **(b).**

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☑ Theme 2 : Characterization and modeling
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Insights into fe-oxidant interactions (N_2O, O_2, CO_2) within FER zeolite frameworks

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Iron-containing zeolites are among the most efficient heterogeneous catalysts for redox processes with high environmental impact, including Selective Catalytic Reduction (SCR) and methane transformation to value added products [1,2]. In this study, we examine the behavior and oxidation dynamics of Fe species embedded in FER zeolite matrix upon interaction with different oxidants (N_2O, O_2, CO_2).

For the study, commercial FER (Tosoh Corporation) with Si/Al 8.5 was selected as a model zeolite material. Iron was introduced by low-level impregnation (<1 wt%) to analyze the changes in oxidation state and local geometry of particular iron species present in FER after interaction with O_2, N_2O, and CO_2. The interactions were monitored under in-situ conditions by Mössbauer, FTIR, and XAS spectroscopies. For samples studied by Mössbauer spectroscopy, ^{57}Fe-precursor was used.

After evacuation of Fe-FER, the Mössbauer and XAS spectroscopic analyses indicate that the material predominantly contains bare Fe(II) species in cationic positions. Upon exposure to the different oxidants, these Fe centers display distinct reactivity patterns. CO_2 induces only limited changes in the oxidation state, although a decrease in local symmetry is observed. In contrast, O_2 promotes partial oxidation, converting roughly 30% of Fe(II) N_2O exhibits the strongest oxidizing effect, leading to complete oxidation of Fe(II) to Fe(III) . For both O_2 and N_2O treatments, an additional spectroscopic contribution is detected on Mössbauer and FTIR spectra, which can be assigned to active oxygen species [1,3]. Such species are known to participate in the oxidation of inert molecules like CH_4, a reactivity of particular interest for low-temperature routes to methane functionalization, for example, the selective conversion of CH_4 to methanol in cyclic activation-extraction processes currently explored for natural-gas valorization [4].

Overall, these results reveal the markedly different oxidizing strengths of the three oxidants ($N_2O > O_2 > CO_2$) and demonstrate the value of Mössbauer spectroscopy as a powerful in situ tool for probing Fe speciation in complex materials such as zeolitic matrices. Moreover, the results obtained from FTIR and XAS methods are complementary to those from the Mossbauer study. This work provides atomic-scale insights into the behavior of Fe-based zeolite catalysts and contributes to a deeper understanding of their role in oxidation reactions.

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THEME

☐ Theme 1 : Synthesis and shaping
☐ Theme 2: Applications for the environment, energy, and health
☒ Theme 3 : Characterization and modeling

Putting ZIF-8 in Shape: ZIF-8 / Polymer Extrudates for Gas Phase Alcohol/Water SeparationsP.

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ZIF-8 is one of the benchmark MOFs for alcohol/water separations owing to its high hydrophobicity and sigmoidal alcohol adsorption isotherm. The gate-opening flexibility of the framework enables molecules such as ethanol (kinetic diameter ≈ 4.3 Å) to penetrate its pores, despite the smaller size of its six-membered ring apertures (≈ 3.4 Å).[1] Since bioethanol is typically produced via energy-intensive distillation (80% of the production cost), ZIF-8 represents a promising alternative adsorbent for ethanol recovery. For practical use, ZIF-8 powder must be formulated with binder to yield mechanically robust and abrasion-resistant structures.[2] Yet, shaping ZIF-8 remains particularly challenging, as the process must preserve all the intrinsic properties of the initial powdered MOF (structural integrity, flexibility, adsorption properties), while the incorporation of binders can profoundly influence, or even compromise, them.

In this work, we developed millimeter-sized ZIF-8 extrudates while preserving their intrinsic framework flexibility. Different binders were screened, using polymeric organic binders (polyvinyl butyral and polyvinylidene fluoride) and cellulose-based binders (methylcellulose, hydroxypropyl cellulose, and carboxymethylcellulose). The shaped materials retained the textural properties and structural flexibility of ZIF-8, as confirmed by nitrogen sorption (77K) and PXRD analyses. As in one of the rare cases in open literature, the mechanical strength of the extrudates was quantified, showing crushing strengths comparable to commercial zeolite pellets and highlighting the strong influence of the binder nature on the mechanical behavior of the composites. Thermogravimetric analysis showed that the formulation process modifies the heat transfer properties of the formulated materials. Selectivity for ethanol over water, based on IAST calculations, showed that, while hydrophobic binders preserved the ethanol-water separation performance of ZIF-8 (with PVDF exhibiting the highest selectivity, α=1 473), hydrophilic binders drastically reduced the selectivity, in some cases reducing it to almost negligible levels. This work highlights how shaping MOFs with organic binders can alter their structural flexibility and, depending on the binder chemical nature, significantly influence their adsorption properties.

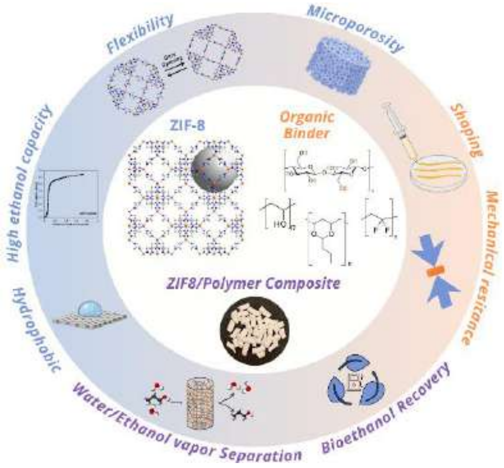

Fig. 1. Graphical abstract

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Neutron diffraction for the localization of coke in zeolite catalysts during methanol-to-hydrocarbons conversion

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The methanol-to-hydrocarbons (MTH) process converts methanol into light olefins and gasoline-range hydrocarbons and provides a non-petroleum route to fuels and key chemical intermediates.[1] A major limitation of MTH is the rapid deactivation due to deposition of high-molecular weight carbon species, which are commonly referred to as coke, formed by secondary reactions that progressively accumulate inside the micropores.

High-resolution constant-wavelength neutron powder diffraction data were collected at HRPT (SINQ, Switzerland) and used to determine the structure of coke species and their location inside deactivated zeolite frameworks. Neutrons are highly sensitive to light elements and provide strong nuclear contrast against the aluminosilicate zeolite framework, which highlights confined hydrocarbon species within porous materials (Fig. 1). This approach made it possible to track the evolution of coke deposits and to establish direct correlations with the catalytic activity of specific zeolite structure.[2,3]

Different medium-large pore zeolite frameworks have been investigated: ZSM-11 (**MEL**), featuring a three-dimensional system of interconnected 10-membered ring channels, ZSM-12 (**MTW**), composed of one-dimensional 12-membered ring channels, and ZSM-22 (**TON**), consisting of narrow one-dimensional 10-membered ring channels. These topological differences strongly influence molecular diffusion, the composition of the hydrocarbon pool, which is governed by the distribution of active sites within the zeolite, and the spatial distribution of coke formation. Neutron diffraction results were correlated with complementary coke quantification techniques (TGA-MS, MAS NMR, FTIR, GC-MS) ensuring consistency between the structural order of coke deposits and their chemical signatures.

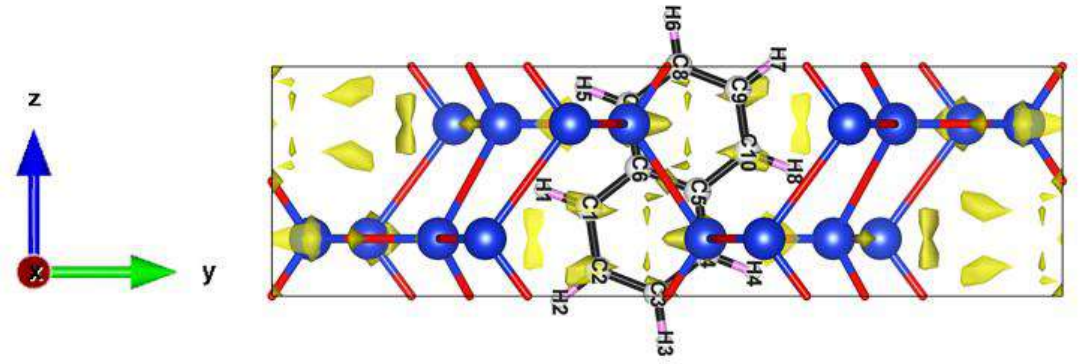

Figure 1. Distribution of coke-related differential nuclear density overlapping with a naphthalene rigid-body model in ZSM-22.

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THEME

☐ Theme 1 : Applications for the environment, energy, and health

☒ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

From Equilibrium to Dynamics: Benchmarking the CO_2 Capture Performance of ZMQ-1

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The rising global energy consumption and continued reliance on fossil fuels are increasing atmospheric CO_2 levels, exacerbating global warming.[1] Efficient carbon capture technologies are essential to decarbonisation efforts. Solid adsorbents such as zeolites stand out as promising materials for this purpose, with the main selection criteria being the adsorption capacity, selectivity, fast kinetics, and stability. With the emergence of ZMQ-1, a new extra-large pore aluminosilicate, we investigate the adsorptive properties of a structure featuring intrinsic intersecting meso-microporous channels, exceptionally high surface area, large pore volume, and excellent hydrothermal stability.[2]

Here we provide a comprehensive evaluation of the adsorption behaviour of ZMQ-1 under static and dynamic conditions compared to that of the intrinsically mesoporous amorphous Al-MCM-41, and the extrinsically mesoporous zeolite USY. ZMQ-1 stands out for its high CO_2 uptake capacity (12.8 mmol/g at 0 °C and 30 bar), outperforming USY and Al-MCM-41. These results are explained by its intrinsic ordered mesoporous channels, which are more accessible than the extrinsic irregular mesopores in USY; for Al-MCM-41, the absence of strong confinement results in lower uptakes. Fractional uptake curves at 0.1 bar as a function of time show that CO_2 adsorption on ZMQ-1 is the fastest, reaching equilibrium in ~82 s, compared to ~212 s and ~333 s for USY and Al-MCM-41, respectively. These results are further supported by ZMQ-1 having the highest Henry's constant, suggesting that at low coverage, it has the strongest affinity for CO_2. Moreover, the almost constant isosteric heat of ZMQ-1 (~20 kJ/mol), is indicative of a homogeneous surface and is in a desirable energy range for efficient use in cycling processes. The high CO_2 adsorption capacity and rapid kinetics of ZMQ-1 are observed during the separation of a simulated biogas stream. Breakthrough curve analysis shows that CO_2 takes the longest time to elute from ZMQ-1 compared to the other materials. In addition, ZMQ-1 exhibited the highest percentage of utilised bed length and the shortest mass-transfer zone among the studied materials, attributed to improved diffusion throughout the porous structure.

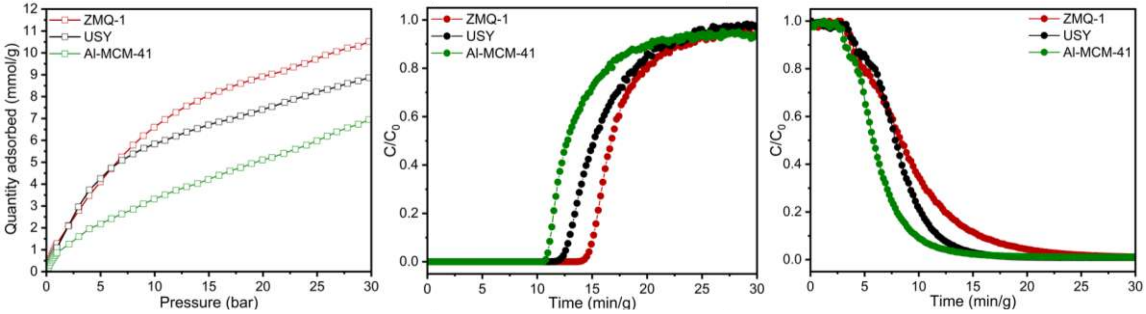

Fig. 1. CO_2 adsorption isotherms (left) breakthrough (middle) and desorption curves (right).

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THEME

☐ Theme 1 : Applications for the environment, energy, and health

☒ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

In-situ heating electron microscopy of metal species in 2D zeolites: tracking metal–support interactions and thermal stability of zeolite-supported catalysts

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Understanding the dynamic behaviour of metal species within zeolitic supports under operating conditions is fundamental to rational catalyst design[1,2]. Here, we employ in-situ heating electron microscopy to directly observe the structural evolution, thermal stability, and localization of supported metal nanoparticles and clusters within zeolitic frameworks. Two-dimensional (2D) zeolites, engineered with abundant surface silanol groups, offer exceptional versatility for anchoring and stabilizing active species at the single-atom and nanoparticle scales. By combining high-resolution scanning transmission electron microscopy (STEM) with correlative SEM–AFM imaging, we capture the real-time behaviour of metal species during thermal activation and reaction conditions, enabling direct description of metal–support interactions.

Our characterization studies reveal how the zeolitic support architecture—particularly the distribution and accessibility of surface silanol groups—governs metal nanoparticle stability, morphology, and reactivity. Through systematic in-situ heating experiments, we identify critical temperature thresholds for nanoparticle sintering and migration, and elucidate how strategic support engineering can mitigate these degradation pathways. We demonstrate that downsized metal catalysts, such as Pt and Pd, supported on 2D zeolites (MWW and MFI topology of layers) exhibit exceptional structural stability under thermal stress while maintaining high catalytic performance.

Furthermore, we explore the incorporation of diverse metal species (Pt, Pd, Co, Ni, *etc.*) *via* the ADOR (Assembly–Disassembly–Organisation–Reassembly) approach[3], exploiting this post-synthetic methodology to create precisely controlled metal–zeolite composites[1]. In-situ observations provide direct insights into how support composition, pore structure, and surface chemistry influence metal clustering behaviour and long-term stability.

This work demonstrates how advanced structural characterization techniques can unlock design principles for robust, thermally stable zeolite-supported catalysts, bridging fundamental materials science with practical catalyst durability.

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Acknowledgments

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

How does structured adsorbent channel heterogeneity influence the efficiency of adsorptive CO2 capture?

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Adsorbent monoliths are becoming the standard in carbon capture applications: they allow to operate at short cycle times and low pressure drop. Commercial monoliths consist of parallel-channel structures, which are extruded through a die. This extrusion process inevitably leads to defects, variations in channel size of 10-20 % are reported in literature.[1,2] The impact of these imperfections on cyclic process performance, is not well understood.

Process simulations were performed to link a distribution in channel sizes to process performance variables in a cyclic vacuum swing adsorption (VSA) process for flue gas carbon capture using zeolite 13X. In a first step, an ideal adsorbent monolith was compared with a fixed bed of zeolite pellets. Using a monolith allows for a higher productivity (0.78 mmol/kgs) compared to a fixed bed (0.68 mmol/kgs) and a lower energy demand (190 kWh /tonne CO_2 versus 320 kWh/tonne CO_2). Furthermore, process performance for monoliths is much less dependent on interstitial gas velocity, allowing a more stable operation with a varying feed gas flow rate.

Next, simulations were performed considering a Gaussian distribution of monolith channel sizes. Simulations were performed with 3σ ranging from 1.2 % to a large variation of 120 %. Starting from a variation of 12 %, a real impact on process performance can be expected. In the worst-case scenario, with a very large channel distribution, recovery drops from 81 % to 68 %, throughput from 0.78 mmol/kg s to 0.65 mmol/kg s and energy demand from 190 kWh / tonne CO_2 to 320 kWh / tonne CO_2 (Figure 1). Interestingly, even for very large wall size distributions, the performance of monoliths remains better than a fixed bed of spherical particles.

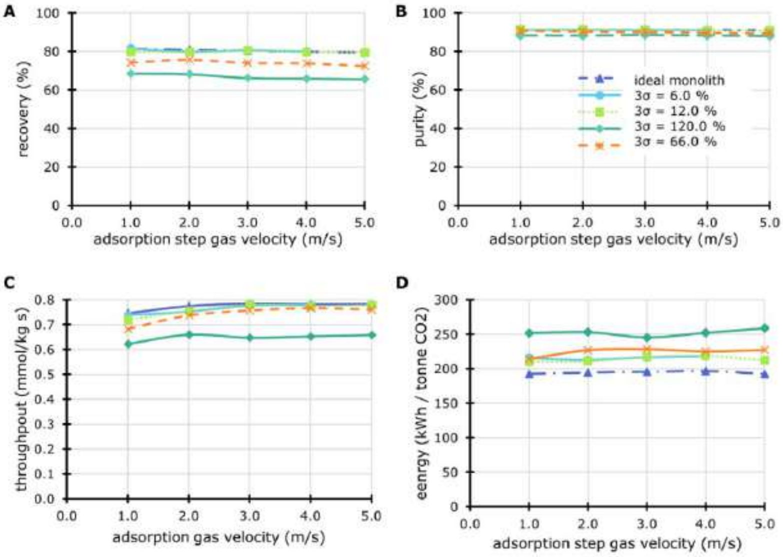

Fig. 1. Comparison between the recovery (A), purity (B), throughput (C) and energy demand (D) of a monolith without wall size distribution and a monolith containing a wall size distribution.

In conclusion, this work shows the promising properties of adsorbent monoliths for CO_2 capture and offers guidelines for practical defect management in structured adsorbents.[4]

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Groupe Français des Zéolithes

GFZ 2026

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Oraux

Thème 3
Applications
(Environnement, énergie, santé)

THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

Développement d'un nouveau protocole de spectrométrie de masse en temps réel dédié à l'optimisation rapide de la pyrolyse catalytique de la biomasse

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La pyrolyse catalytique rapide (FCP) de la biomasse lignocellulosique conduit à l'obtention de bio-huiles contenant des molécules plateformes, parmi lesquelles le benzène, le toluène, l'éthylbenzène et les xylènes (BTEX). Classiquement, la démarche employée pour l'optimisation consiste à produire une bio-huile en réacteur pour chaque condition catalytique, puis à l'analyser dans un second temps. Les méthodes analytiques utilisées emploient généralement des systèmes chromatographiques en phase gazeuse ou liquide, souvent couplés à la spectrométrie de masse (GC ou LC-MS) ou bien des spectromètres de masse à très haute résolution (HRMS) [1,2]. Cette approche en deux temps est longue et peut introduire des biais (récupération des composés dans un solvant, rétention de fractions). Elle ne permet pas non plus une caractérisation fine avec un suivi temporel des réactions catalytiques. Afin d'accélérer l'optimisation de la FCP, nous avons développé une méthodologie haut débit d'analyse directe par HRMS des produits de pyrolyse catalytique en lit fixe, permettant, en quelques minutes, d'examiner l'ensemble des molécules formées pour une condition de pyrolyse catalytique donnée (catalyseur, biomasse, température) (Figure 1a.). Afin de valider cette nouvelle approche, nous avons étudié les produits de pyrolyse de la cellulose en employant des catalyseurs de structure **Zeolite Socony Mobil Five (ZSM-5),** bien connues dans la littérature [3,4]**.** Les résultats obtenus à l'aide de cette nouvelle méthodologie permettent de reproduire les résultats déjà reportés (Figure 1b., Figure 1c.), ouvrant la voie à une étude approfondie et haut débit d'un large éventail de conditions de pyrolyse catalytique.

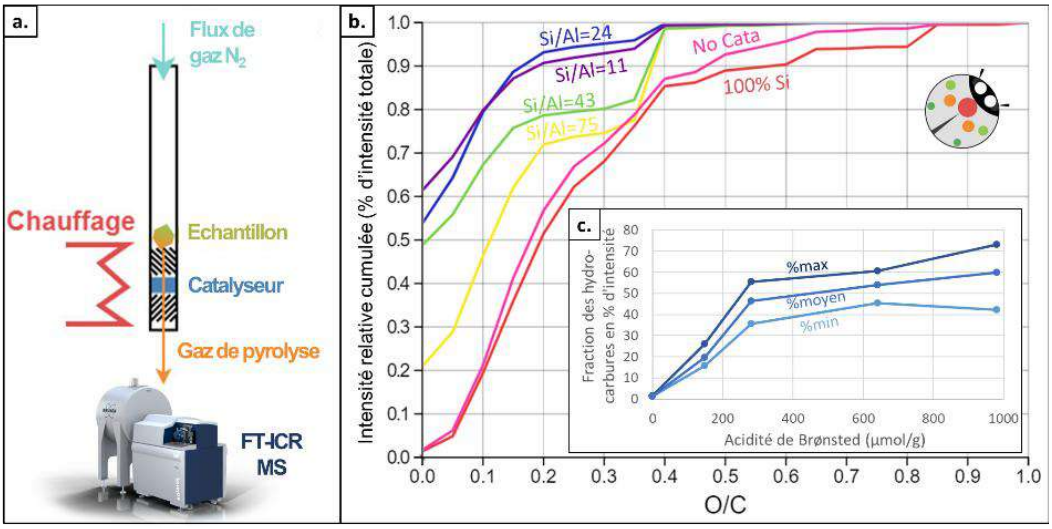

Figure 1 : a. schéma du principe de la méthode DIP-APCI FT-ICR MS. Evolution **b.** de l'intensité relative cumulée des produits de pyrolyse de la cellulose en fonction de leur rapport O/C et du catalyseur et, **c.** de la fraction d'hydrocarbures en fonction de l'acidité de Brønsted.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

Encapsulated iron oxide nanoparticles within the intrawall pores of SBA-15 via melt infiltration as efficient Fenton-like catalyst for lindane degradation

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Abstract

The efficient degradation of lindane, a persistent organic pollutant, remains a major challenge for advanced oxidation processes (AOPs), particularly in Fenton-type systems that employ heterogeneous catalysts, the effectiveness remains often hindered by nanoparticle aggregation, poor mass transfer, and iron leaching [1]. To address this challenge, we developed iron-based catalysts using a melt infiltration (MI) strategy with an additional time-controlled diffusion step to embed Fe_2O_3 nanoparticles within the intra-wall pores (IWP) of SBA-15 mesoporous silica. Physicochemical analyses (XRD, N_2 physisorption, DR UV-Vis, HR-TEM and synchrotron PDF) revealed that prolonged infiltration leads to the selective placement of well-dispersed hematite nanoparticles (<3 nm) exclusively in the IWP region, while the SBA-15 support retains its mesostructural integrity and porosity (fig. 1) [2]. Catalytic tests in the Fenton-like oxidation revealed a notable improvement in lindane removal, with degradation efficiency increasing from 54% to reaching 91% in optimized samples. This performance was achieved after 240 minutes at pH 3 and 50 °C, with iron leaching kept below 2 ppm, significantly lower than values reported for similar systems. Control experiments confirmed that heterogeneous H_2O_2 activation at the solid–liquid interface dominates over homogeneous pathways, with confined nanoparticles ensuring efficient radical utilization. These findings demonstrate that melt infiltration (MI) strategy with an additional time-controlled diffusion step is an effective strategy for stabilizing iron oxide nanoparticles while tailoring the reaction microenvironment to enhance catalytic performance. Beyond its application to lindane oxidation, this strategy presents a flexible, broadly applicable pathway for creating robust, high-efficiency catalysts suited for advanced oxidation of persistent organic pollutants.

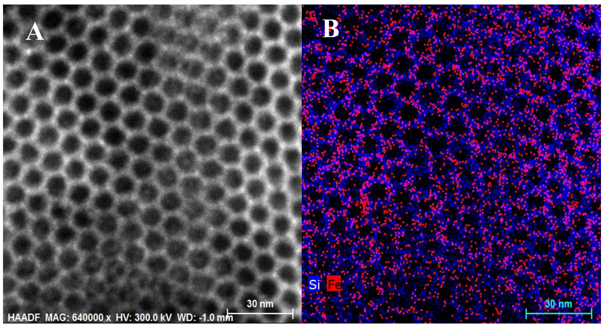

Fig. 1. HAADAF S/TEM image (A) and EDXS distribution of Si-(blue) and Fe-(red) elements (B) for the 10Fe_4 catalyst.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Exploring Dendritic Zeolites as Catalytic Supports for Ethylene Oligomerization

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Heterogenization of homogeneous Ni(II) complexes is an effective strategy to combine the high catalytic performance of molecular systems with the stability and reusability of heterogeneous solids. In this way, dendritic MFI zeolites arise high interest due to their outstanding accessibility [1].

In this work, we report the anchoring of a nickel 2,2′-dipyridylamine (*dpa*) complex onto MFI-type zeolitic supports with tailored morphologies and compositions, with emphasis on dendritic MFI materials (Fig.1). The *dpa* ligand was covalently grafted onto the support via silanization, followed by complexation with nickel [2]. A variety of zeolitic supports (Al-MFI(d), Cu-Al-MFI(d), and mesoporous Cu-MFI) were synthesized with controlled Si/Al ratios (25, 30, and 40) and heteroatom content prior to heterogenization [3]. The materials were characterized by XRD, Ar physisorption, ^{29} Si MAS NMR, TGA, CHN, ICP-OES, SEM, and TEM. The results confirmed successful covalent anchoring of the ligand, preservation of MFI crystallinity, and maintenance of hierarchical porosity. Catalytic tests employing ethylaluminium sesquichloride (EASC) as co-catalyst revealed that [Al-MFI(d)(25)-Ni] combines high activity and enhanced selectivity toward C_4 and α-C_4 , matching or even surpassing the homogeneous precursor under comparable conditions. Performance trends demonstrate a strong support–structure relationship: lower Si/Al ratios (higher acidity) increase catalytic activity, while dendritic morphology improves accessibility and promotes α-olefin formation. Cu-containing dendritic supports exhibit a synergistic enhancement in activity without significant loss of selectivity when compared to reference supports with similar Si/Al ratio. In addition, the XRD pattern of the [Al-MFI(d)(25)-Ni] catalyst after reaction confirmed the preservation of the zeolite's dendritic structure and crystallinity.

Overall, these results demonstrate that covalently anchored Ni(*dpa*) complexes on dendritic MFI supports are promising, tunable precursors for selective ethylene oligomerization.

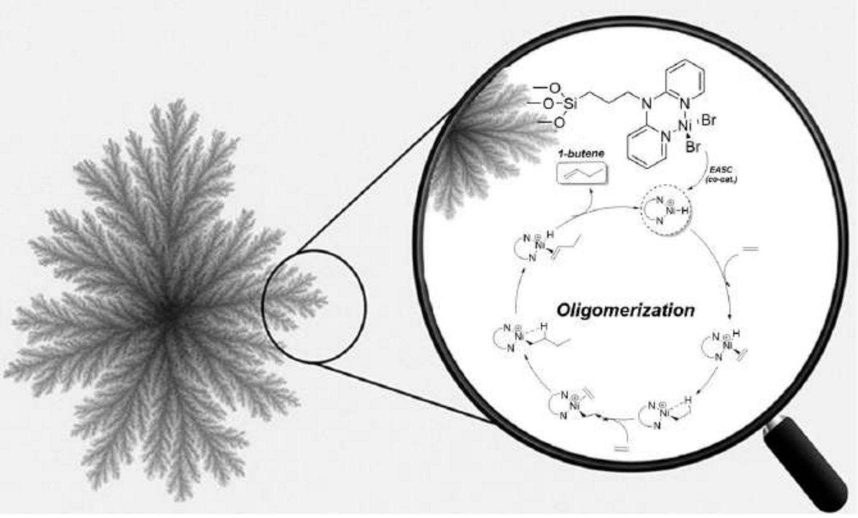

Fig. 1. Schematic representation of the catalytic precursor heterogenized on a dendritic zeolite.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

MIL-160: A Sustainable Adsorbent for Water Harvesting and Adsorption Cooling Technologies

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MIL-160 is a hydrothermally stable and scalable aluminum MOF exhibiting high performance in water adsorption–desorption cycles relevant to adsorption chillers and atmospheric water harvesting. Compared to the commercial benchmark FAM-Z02,**[1]** MIL-160 shows similar adsorption isotherm shapes and uptake at comparable relative pressures, while delivering a substantially 70% improvement in working capacity (170 mg g^{-1} versus 100 mg g^{-1}), making it more effective for cooling applications.

Breakthrough experiments reveal similar S-shaped breakthrough curves for both materials but confirm the superior uptake of MIL-160. Its key advantage lies in desorption performance during cycling: at 60 °C, a temperature accessible from waste heat. At this temperature, MIL-160 releases 80% of its adsorbed water, enabling a cycling sorption capacity of 16.2 mmol g^{-1} with stability over repeated cycles. In contrast, FAM-Z02 desorbs only 60% of its adsorbed water, corresponding to 9.5 mmol g^{-1}. Increasing the regeneration temperature to 80 °C enhances the cycling performance of FAM-Z02 to 76% (12 mmol g^{-1}), yet this remains lower than the regenerated capacity of MIL-160 at 60 °C. Furthermore, the composition of MIL-160, based on abundant and low-toxic aluminum, available and biosourced FDCA linker, combined with a green synthesis route, makes it highly suitable for large-scale production.**[2]** The combination of enhanced adsorption capacity, efficient regeneration, and a green synthesis route highlights the strong potential of MIL-160 for water harvesting technologies.

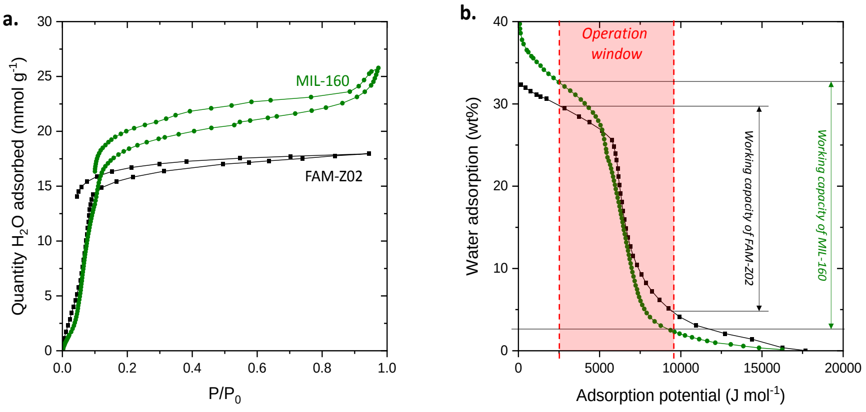

Fig. 1. Water adsorption isotherms of FAM-Z02 (black squares) and MIL-160 (green circles) performed at 20 °C (a), and resulting water uptake as a function of the adsorption potential (b).

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THEME

☒ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Impact du Cérium sur l'adsorption de diiode gazeux et sa conversion dans des Metal-Organic Frameworks de type UiO-66

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Le radioisotope ^{131}I, formé lors d'accidents nucléaires, induit des risques de cancer de la thyroïde [1, 2]. Dans le but d'empêcher sa dispersion dans l'air, par exemple en cas d'explosion d'un réacteur nucléaire, l'adsorption de l'iode 131 est donc un enjeu de santé publique. La conversion d'espèces volatiles de l'iode (comme I_2) en espèces non volatiles (telles que I_3^-) permet ensuite de piéger l'iode converti [3]. Dans ce contexte, les matériaux présentant à la fois une microporosité structurale et une activité catalytique, tels que les Metal-Organic Frameworks (MOFs) et les zéolithes, sont particulièrement intéressants pour cette application. Cette étude décrit l'adsorption et la réactivité du diiode dans des MOFs UiO-66 (Zr/Ce) et s'intéresse au rôle spécifique du cérium comparé au zirconium, lié à son comportement redox et ses propriétés électroniques particulières.

Des mesures de DRX sur poudre ont permis de confirmer l'obtention d'UiO-66 (Zr_xCe_{1-x}) avec x = 0 ; 0,25 ; 0,5 ; 0,75 et 1 en phase pure. L'incorporation du cérium est qualitativement confirmée par une augmentation progressive du paramètre de maille avec la fraction molaire de cérium utilisée en synthèse (causée par la plus grande taille de Ce^{4+} par rapport à Zr^{4+}). Les MOFs synthétisés ont ensuite été mis en contact avec un mélange $Ar/^{127}I_2$, montrant une adsorption de I_2 allant de 54 à 206 mg/g après 16 heures de contact. Nos résultats montrent que l'augmentation de la proportion de cérium diminue l'adsorption de I_2 dans les UiO-66 étudiés. Des expériences de spectroscopie Raman, conduites après adsorption, ont permis d'identifier 3 espèces de l'iode, à savoir I_2, $[I\text{-}I]_n\text{-}I^-$ et I_3^-. En exploitant cette information, il apparait que la conversion de I_2 en I_3^- est inhibée par la présence de Ce dans le MOF. Cela pourrait être dû à la conversion facile de Ce^{4+} en Ce^{3+}, éventuellement accompagnée d'une reconversion du I_3^- formé en I_2.

Cependant, diverses études [4, 5] ont mis en évidence la coexistence de Ce^{4+} et Ce^{3+} en proportions non négligeables dans le MOF UiO-66 (Ce). Cette observation conduit à se demander s'il est possible de sélectivement faciliter les conversions de Ce^{3+} en Ce^{4+} pour des applications en réduction (par exemple la conversion de I_2 en I_3^-) ou de Ce^{4+} en Ce^{3+} pour des applications en oxydation (afin par exemple de dégrader des polluants organiques). Afin de répondre à cette question, des travaux sont en cours concernant la fonctionnalisation des ligands de l'UiO-66 par des groupements $-NH_2$ et $-NO_2$.

Les UiO-66 (Zr/Ce) synthétisés ont ainsi montré une adsorption de I_2 gazeux ainsi qu'une conversion de I_2 vers I_3^-, permettant de limiter la volatilité de l'iode piégé. L'incorporation de Ce dans l'UiO-66 (Zr) montre un effet sur les propriétés d'adsorption et de conversion de l'iode, qui pourrait être causé par les propriétés redox du cérium. Des caractérisations supplémentaires par RPE, MEB, XPS et adsorption d'azote sont en cours, de même qu'une fonctionnalisation des MOFs ayant pour objectif de contrôler le comportement redox du cérium dans les matériaux obtenus.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

Plastic Pyrolysis over Extra-Large Pore Zeolites

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Global plastic pollution is projected to reach 66.1 million tons per year by 2050 under a business-as-usual scenario.[1] Combined with the continued reliance on non-renewable petroleum resources and the non-biodegradability of plastics; this trend underscores the urgent need for efficient strategies to valorize and upgrade plastic waste. Catalytic pyrolysis has emerged as a promising pathway to convert plastic waste into valuable hydrocarbons,[2] with zeolites attracting attention due to their well-defined porosity and Brønsted acidity.[3] While medium and large pore zeolites have been widely studied,[4] recent advances in extra-large pore structures such as **ZEO-1** (JZO-type)[5] with 16 membered ring channels and **ZMQ-1**[6] featuring 28 membered ring mesoporous openings offer improved molecular accessibility for bulky polymer chains.

This work investigates the catalytic performance of extra-large pore zeolites **ZEO-1** and **ZMQ-1** with crystalline structures and morphologies verified by XRD and SEM (Fig. 1) for the pyrolysis of low-density polyethylene (LDPE), benchmarking them against **ZSM-5**, **CBV-760**, and the non-zeolitic mesoporous material **MCM-41**. The catalysts exhibit micropore volumes of 0.10 to 0.31 cm³/g, mesopore volumes of 0.10 to 0.36 cm³/g, and BET surface areas between 500 and 1000 m²/g.

Catalytic pyrolysis experiments were conducted in a fixed-bed reactor under a nitrogen flow rate of 20 mL/min, using a polymer-to-catalyst ratio of 1. Gaseous and liquid products were analyzed online by GC-MS, and coke deposits were quantified using thermogravimetry (TGA). Pyrolysis at 375 °C shows that all catalysts significantly outperform catalytical pyrolysis, achieving 80 to 99 percent LDPE conversion. Importantly, the extra-large pore zeolites demonstrate superior stability across multiple reaction cycles compared to **MCM-41**. Their combination of high conversion efficiency, favorable hydrocarbon selectivity, and strong catalytic durability positions extra-large pore zeolites as highly promising materials for the efficient upgrading of polyethylene waste.

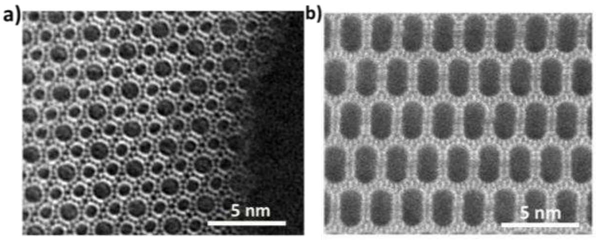

Fig. 1 | The structures and STEM images. a, Calcined **ZEO-1**. b, Calcined **ZMQ-1**.

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Real time tracking of Gallium oxides in MFI zeolites during reaction by operando approaches

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Nowadays, the production of high value-added chemicals (HVC) is limited to two technologies: catalytic reforming and steam cracking of naphta. Among alternative technologies, propane aromatization stands out for its commercial potential. Gallium-doped zeolites represent a promising class of catalysts for this process [1-2]. We therefore sought robust methodologies to gain deeper insight into both the catalyst properties and the reaction process. To this end, an operando approach based on FTIR spectroscopy was adopted. Operando FTIR measurements were carried out over a temperature range from 25 °C to 530 °C using a dedicated high temperature IR reactor, commonly referred to as a sandwich cell, specifically designed for operando investigations under reaction conditions.

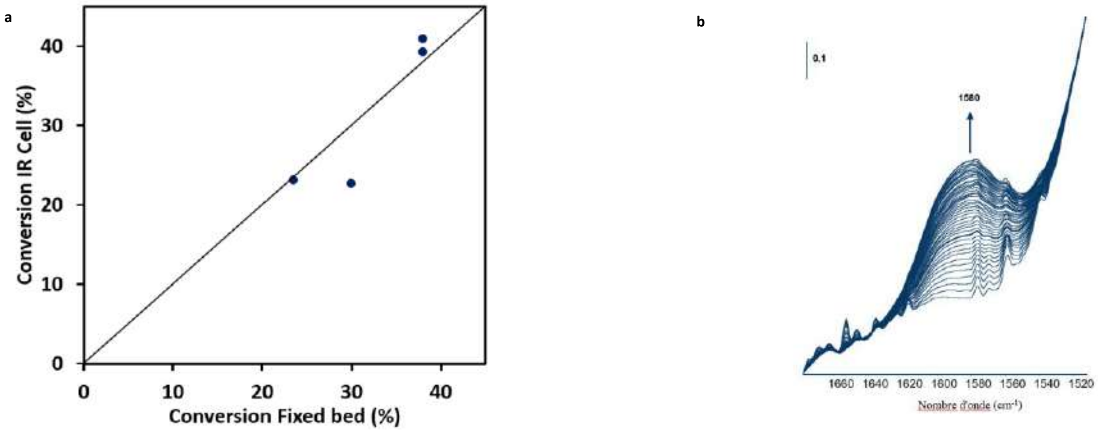

Figure 1. (a) Propane conversion obtained under conventional catalytic conditions determined by Gas chromatography (GC) at 530 °C as a function of the propane conversion determined by Infrared spectroscopy (IR) in the sandwich cell. (b) Evolution of the amount of coke formed on the catalyst during the reaction.

In **figure 1-a** the reaction performed using the sandwich cell yields results comparable to those obtained under conventional catalytic conditions in a fixed-bed reactor, thereby confirming the reliability of the reactions conducted in this reactor configuration. In addition, this cell enables in situ monitoring of coke formation during the reaction, as illustrated in **Figure 1-b** by the progressive increase of a band at 1580 cm^{-1}, which correlates with the decrease in catalytic conversion over time.

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Posters

Thème 1

Synthèse et Mise en Forme

THEME

☐ Theme 3 : Synthesis and shaping

A mixed-ligand strategy to enhance MOF stability and functionality: Case study on copper MOFs and CO_2 adsorption

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A mixed-ligand strategy was employed to design copper-based metal–organic frameworks (MOFs) with controlled structural stability and CO_2 adsorption properties.[1] Two pillared-layer MOFs were synthesized by combining 2,5-thiophenedicarboxylic acid (TDC) with neutral N-donor ligands, pyrazine (Pyr) and 1,4-diazabicyclo[2.2.2]octane (DABCO). Cu(II), positioned between hard and soft acids according to Pearson's HSAB theory, was selected to enable coordination with both carboxylate and nitrogen-based ligands.[2] Structural analysis by single-crystal X-ray diffraction shows that the Cu–TDC–DABCO system forms a layered framework stabilized by hydrogen bonding between adjacent sheets (Fig.1.), whereas Cu–TDC–Pyr adopts a more compact 3D architecture. Both materials undergo irreversible structural transformations above ~200 °C, as evidenced by PXRD and thermogravimetric analyses.

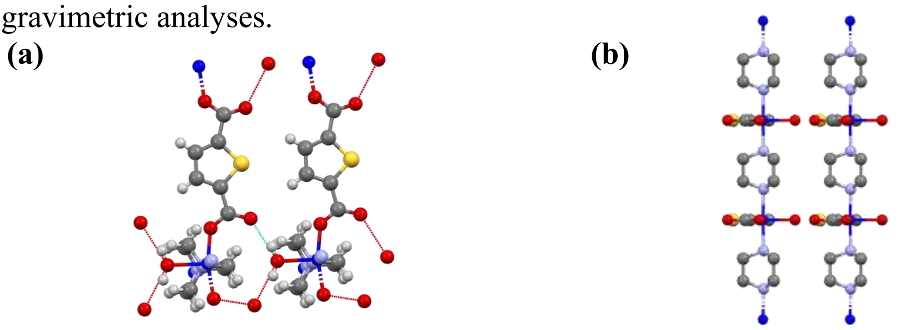

Fig.1. (a) View of the two-dimensional pillared-layer network of Cu–TDC–DABCO, highlighting hydrogen-bonding interactions between adjacent layers (cyan dashed lines). **(b)** View along the b-axis showing the layered architecture formed by 2,5-thiophenedicarboxylate linkers and DABCO pillars. Colour code: Cu = blue, O = red, C = grey, S = yellow. Hydrogen atoms are omitted for clarity.

CO_2 adsorption measurements at 273 K and up to 1.2 bar reveal that Cu–TDC–DABCO adsorbs up to 2.5 mmol g^{-1} after activation at 120 °C. This uptake can be attributed to the presence of accessible confined pores created by the pillared-layer arrangement, combined with polar adsorption sites arising from exposed carboxylate oxygen atoms and heteroatoms within the thiophene rings.[3] In addition, hydrogen-bond-stabilized interlayer spacing likely promotes favourable host–guest interactions while maintaining pore accessibility. Upon activation at higher temperature (200 °C), a decrease in CO_2 uptake is observed, consistent with partial structural rearrangement and reduced accessible porosity. In contrast, the Cu–TDC–Pyr framework shows limited CO_2 adsorption, which is consistent with its low N_2-accessible porosity and dense framework packing. These results illustrate how ligand choice and secondary interactions influence pore accessibility and gas adsorption behaviour in copper-based mixed-ligand MOFs.[4]

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THEME

☐ **Theme 1 : Applications for the environment, energy, and health**
☐ Theme 2 : Characterization and modeling
☒ Theme 3 : Synthesis and shaping

Mixed Valence HKUST-1 As an Heterogenous Catalyst for Click Reaction (CuAAC): A Comparative Study

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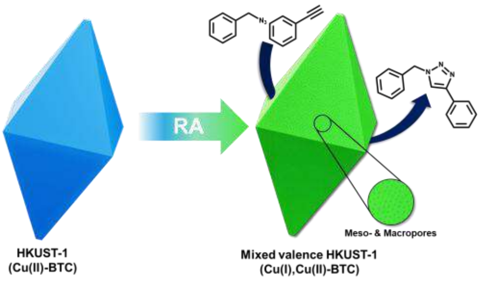
Abstract

Metal–organic frameworks (MOFs) are porous materials formed by the self-assembly of metal ions and organic linkers. They have attracted significant scientific interest and were recognized with the 2025 Nobel Prize due to their wide-ranging applications [1]. A well-studied example is HKUST-1, which is constructed from copper(II) ions and 1,3,5-benzenetricarboxylic acid [2]. However, the inherent microporosity of MOFs limits their use in catalysis involving large molecules. On the other hand, the Copper-Catalyzed Azide–Alkyne cycloaddition (CuAAC) is highly valuable in pharmaceutical synthesis. It typically relies on homogeneous copper catalysts generated in situ from copper salts and reducing agents (e.g., Ascorbic Acid) [3]. However, homogeneous systems are impractical for large-scale applications due to economic and environmental concerns, driving the search for stable, heterogeneous alternatives.

This study presents a novel approach: the post-synthetic reduction of Cu^{2+} in HKUST-1 to catalytically active Cu^{+} using various reducing agents, namely $NaBH_4$, Hydroquinone, Hydrazine, Phenylhydrazine, Ascorbic Acid, and metallic Lithium, at Cu:reductant molar ratios ranging from 1:0.1 to 1:100. This treatment not only generates mixed-valence Cu(I)/Cu(II) sites but also introduces hierarchical porosity (meso- and macropores), thereby enhancing reactant diffusion. Catalytic screening in the CuAAC reaction between Phenylacetylene and Benzyl Azide at 80 °C for 3 hours showed that untreated HKUST-1 exhibited negligible activity. In contrast, reduced variants, particularly those treated with Hydrazine, achieved conversions exceeding 99% at reductant ratios of 1:5 or higher. Even at a lower temperature of 60 °C, Hydrazine-treated catalysts delivered high conversions (84–91%). However, catalyst stability varied: the material prepared at a 1:100 ratio deactivated after a single cycle (yielding only 19% conversion in the second cycle and trace amounts in the third), whereas those treated at 1:5 and 1:10 ratios retained their activity over multiple cycles.



RA=$NaBH_4$, hydroquinone, hydrazine, phenylhydrazine, ascorbic acid, or metallic lithium.

Fig. 1. Mixed-valence HKUST-1 as an heterogeneous catalyst for CuAAC reaction

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☒ Theme 3 : Synthesis and shaping

Synthesis of NMC-MOFs from spent lithium-ion battery cathodes: Comparison of Sonochemical and Mechanochemical routes

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Abstract

End-of-life lithium-ion batteries represent both a sustainability challenge and a valuable source of critical metals [1]. We present a direct upcycling strategy that converts spent Ni–Co–Mn (NCM) cathodes into multimetal metal–organic frameworks (MOFs) using two distinct energy-driven routes: sonochemical and mechanochemical synthesis [2]. Both methods yield crystalline, phase-pure NiCoMn MOFs while retaining the parent cathode's multi-metal composition, yet they differ in efficiency and scalability[3]. Sonochemical synthesis harnesses acoustic energy to rapidly nucleate and assemble frameworks, achieving fast crystallization within minutes. In contrast, mechanochemical processing relies on mechanical impact to drive bond formation, drastically reducing solvent use and offering superior scalability for bulk production [4], [5]. The resulting MOFs exhibit decent porosity and strong CO_2 adsorption test using two different temperature conditions 273.15 K and 297.15 K, comparable to benchmark MOFs prepared from commercial precursors. By contrasting the speed of sonochemical synthesis with the solvent economy and scalability of mechanochemical processing, this work establishes acoustic and mechanical energy as complementary drivers for sustainable porous material synthesis and battery waste valorization.

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THEME

☐ Theme 1 :Applications for the environment, energy, and health
☐ Theme2 :Characterization and modeling
X Theme 3 : Synthesis and shaping

Synthesis of Zeolites from natural clay: Study of synthesis parameters

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This project focuses on the valorization of Tunisian clays, particularly the smectite from Gabès (south of Tunisia), illite from Tataouine (South of Tunisia), and kaolin from Sejnane (North of Tunisia), for the synthesis of zeolites. Zeolites, which are microporous aluminosilicates, possess unique properties that make them highly effective for adsorbing pollutants, including volatile organic compounds (VOCs) such as toluene.

The study aims to optimize three key parameters in the zeolite synthesis process: the type of clay used, the NaOH-to-clay ratio, and the crystallization time. Results indicated that smectite, with an optimal ratio of 1.6 and a crystallization time of 24 hours, leads to the production of Faujasite X zeolite characterized by high purity and crystallinity. Additionally, it exhibits cation exchange capacities of 365 meq/100 g and a specific surface area of 425.4 m^2/g. In additional, Illite also produces pure Faujasite X zeolite with ratio NaOH/Clay = 1.4 and a 24 hours of crystallization, while kaolin (R= 1 and time of crystallization = 24h) results in a zeolite containing two phases, X and LTA, making it less effective for adsorption applications.

Adsorption tests demonstrated that the synthesized zeolites out perform the clays in terms of adsorption efficiency, with significant performance noted for samples prepared from Smectite and Illite. Analysis of isotherms and kinetic models confirmed that the adsorption process follows a pseudo-second-order mechanism, indicating monolayer adsorption on a homogeneous surface. Moreover, the treatment of industrial effluents achieved toluene retention rates of up to 98%.

Keywords: Clay, zeolite, adsorption, Toluen.

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THEME ☒ Theme 1 : Synthesis and shaping

Zeolite GIS polymorphs derived from clay fraction >2 µm: The ability of clay fraction >2 µm for crystallization of high-purity Na-P1 zeolite

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Abstract

Both Si and Al in clay fraction >2 µm (Cf>2µm) of natural bentonite, volclay, was utilized for fabrication of low-cost zeolite, which can be used in large scale of industry.

This study focuses on the fabrication of single-phase gismondine-Na type P zeolite (GIS-NaP) from Cf>2µm by hydrothermal treatment. The Cf>2µm was activated via alkaline fusion at 750°C in a ratio of 1: 1.2, Cf>2µm: NaOH. Pure crystalline GIS-NaP zeolite was successfully produced in a single step through a hydrothermal activation of the supernatant at 150°C, which result from a water treatment of the fusion-Na-Cf>2µm in a ratio of 1: 4, fusion-Na-Cf>2µm: H2O.

The Cf>2µm was identified by X-Ray diffraction (XRD). The supernatant was analyzed via Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES). The synthetic products were characterized with XRD, scanning Electronic Microscopy (SEM), Energy Dispersive and Fourier Transform Infrared spectroscopy (EDS and FT-IR) methods.

The 18 hours were sufficient that a high ordering crystallinity P1 polymorph was formed under Si/Al ratio: 1.47. The zeolite Na-P1 content is found to obviously increase with increasing hydrothermal time from 18h to 36h, so that the climax of Na-P1 zeolite crystallization is reached at 36h, with Si/Al ratio: 1.34. The N2 adsorption indicates the mesoporous character of Na-P1 at the climax, with BET surface area and pore size of 41.76$\mathrm{m}^2.\mathrm{g}^{-1}$ and 8.2nm, respectively. Additionally, the polymorph P2 with Si/Al ratio around 1.81 was spontaneously formed after 6 days of crystallization (interzeolitic transformation) from the same supernatant.

These results provide an experimental basis for the use of the clay fraction >2 µm for the synthesis of zeolites P, which may be useful in the future.

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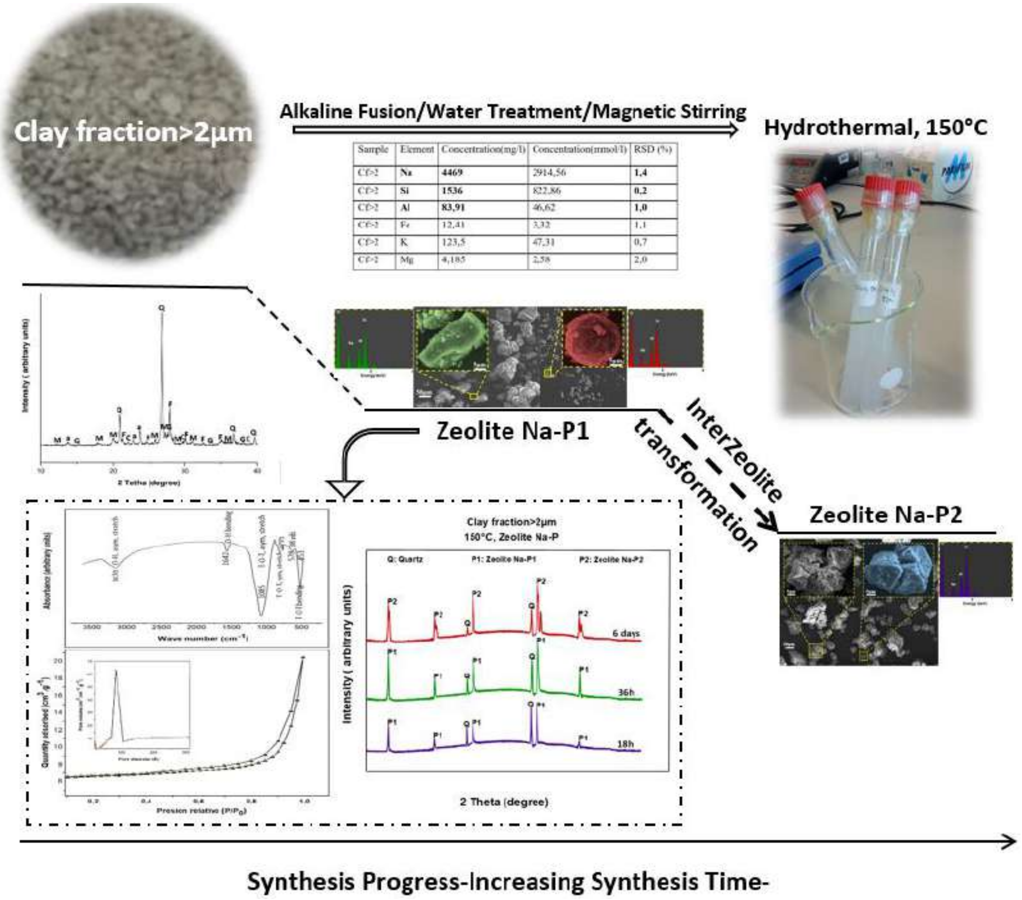

Sample	Element	Concentration(mg/l)	Concentration(mmol/l)	RSD (%)
Cf>2	**Na**	**4469**	2914,56	**1,4**
Cf>2	**Si**	**1536**	822,86	**0,2**
Cf>2	**Al**	**83,91**	46,62	**1,0**
Cf>2	Fe	12,41	3,32	1,1
Cf>2	K	123,5	47,31	0,7
Cf>2	Mg	4,185	2,58	2,0

THEME

☐ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☒ Theme 3 : Synthesis and shaping

Synthesis and characterization of MFI-type zeolites containing Al and/or Ti heteroatoms into the framework

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Zeolite properties can be tuned by the isomorphous substitution of silicium at tetrahedral sites (T sites) of the framework by different trivalent or tetravalent atoms. Typically, Si^{IV} is substituted by Al^{III}, forming Brønsted acid sites, but other heteroatoms have been investigated, such as Ti^{IV}, leading to the creation of Lewis acidity[1]. From the theoretical point of view, Si/Al ratios above 1 are required to obtain a stable framework, according to the Löwenstein's rule. **MFI**-type zeolites in particular, are widely used in catalytic applications due to their high thermal stability and molecular sieve properties. Interestingly, **MFI** frameworks can accommodate a large variety of elemental compositions at T sites including purely silicic (silicalite-1), aluminosilicic (ZSM-5) and titanosilicic materials (TS-1). From experimental data, previous works have shown that Al^{III} and Ti^{IV} can be incorporated at tetrahedral positions in **MFI** frameworks with Si/Al and Si/Ti ratios down to 10 and 40 respectively[1,2]. For TS-1, the use of Si/Ti ratios below 40 in the synthetic gel leads to the co-formation of extraframework titanium oxide species, which are reducing catalytic performances[3]. Al,Ti-ZSM-5, containing both heteroatoms, has also been developed to study its catalytic performances.

In this study, **MFI**-type zeolites containing aluminium and/or titanium heteroatoms were synthesized via a hydrothermal route following reported protocols[4], targeting Si/Al and Si/Ti ratios of 70 to maximize heteroatoms insertion into the framework. The resulting materials were characterized by XRD, XRF, N_2 physisorption and SEM-EDX (Fig. 1).

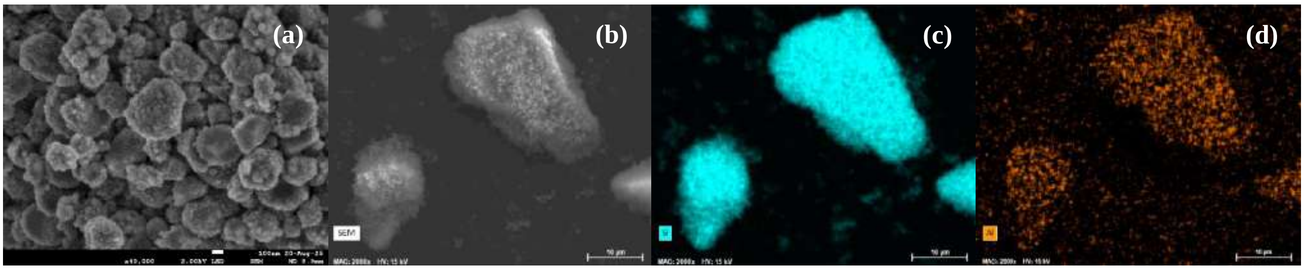

Fig. 1. *SEM images (×40,000 magnification) of (a) Al-ZSM-5 ; SEM images of selected areas for EDX analysis (×2,000 magnification)(b), and elemental maps showing the distribution of (c) Si and (d) Al.*

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modelling
☒ Theme 3 : Synthesis and shaping

Metal Encapsulation in Zeolites: From Robotic Synthesis to Catalytic Function

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Robotic synthesis provides a powerful approach for the controlled encapsulation of metal species within zeolites, enabling precise and reproducible control over key synthesis parameters governing metal incorporation.

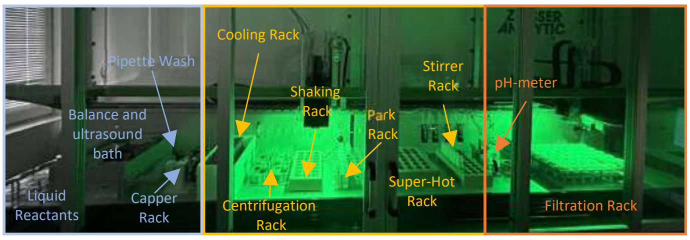
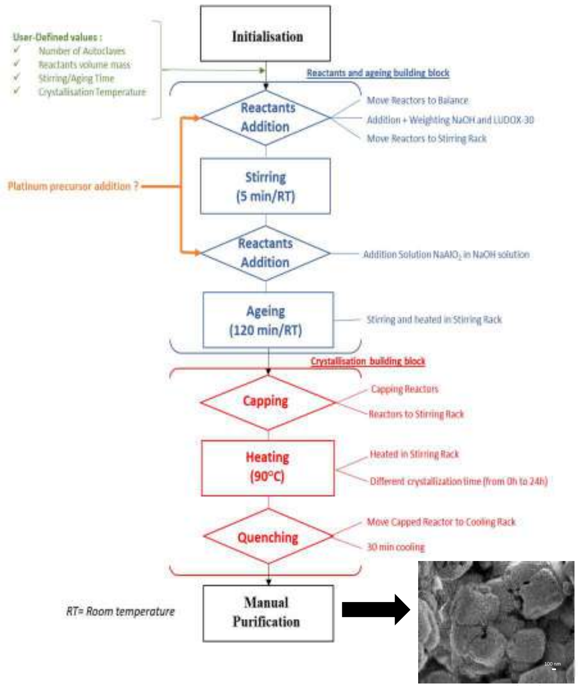


Fig 1: Pictures of Synthesis Platform with the different racks

To optimize these architectures, synthesis protocols for bifunctional zeolites have been developed using a high-throughput robotic synthesis platform separated in several blocks (Fig.1) including Reactants Handling or Crystallization as example. Two arms allow movements for pipetting or handling reactors and autoclaves. These protocols are implemented through a SQL-like programming language, allowing precise control over robotic parameters and a significant reduction of experimental uncertainties, such as pipetting speeds and volumes, as well as independent programming of individual reactors through predefined sequence combinations. This approach enables systematic exploration of a broad formulation space by tuning addition kinetics, concentration profiles, crystallization times, and hydrothermal conditions, while substantially reducing development costs and timescales.



LTA morphology

Fig. 2: LTA-Synthesis Programming Diagram

Within the **ANR H2RECOVER** project, these strategies are applied to the encapsulation of platinum in low-porosity zeolites, with a particular focus on the LTA structure. Following the development of a reference manual synthesis[1], the protocol was successfully transposed to the robotic platform through dedicated program coding (Fig. 2). Beyond synthesis optimization, the robotic approach provides a powerful framework for investigating synthesis-gel phase diagrams, crystal growth mechanisms, and alternative pathways for platinum incorporation. The synergistic interaction between platinum and the zeolite framework has already demonstrated promising performance in the gas-phase hydrogenation of organic compounds[2]. In the case of LTA, this synergy further enables hydrogen gas separation by adsorption, achieved through porosity reduction via cation exchange within the α-cages.

Overall, the combination of zeolitic confinement, cation-controlled porosity, and automated synthesis methods provides a highly effective route for the design of structurally well-defined zeolites, addressing current challenges in catalysis for hydrogen valorization and transport.

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sTHEME

☐ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☑ Theme 3 : Synthesis and shaping

Influence of NaX with different crystal sizes on the conversion of glycerol-to-glycerol carbonate

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Recently, glycerol carbonate (GLC) produced by heterogeneous catalysts has been developed, and stability and reusability remain key to achieving a sustainable process by using porous zeolite [1]. In a previous study [2], glycerol carbonate was produced from glycerol and dimethyl carbonate over Na-based zeolites, including Beta, LTA, ZSM-5, and NaY. Only the NaY zeolite exhibits high yield, selectivity, and stability. There is a similar zeolite type, NaX, with higher basicity that directly exhibits high sodium cation content. Therefore, the use of NaX zeolite as a catalyst enhances basicity and catalytic activity. Moreover, it compared the effect of NaX morphology size. The catalysts were characterized using XRD, SEM, FTIR, and N_2 sorption analysis. The SEM images in Figure 1 show NaX crystal sizes ranging from approximately 0.7 to 2.0 µm. The GLC conversion, selectivity, and yield were analyzed by HPLC/RID. The GLC yield of the small-sized NaX_07 is 75% from a 2 h reaction time and 100% selectivity. In contrast, the larger NaX_2.0 yields 68% under the same conditions. The results show that NaX with small crystal sizes exhibits higher activity and greater reactant diffusion to the zeolite catalytic site, resulting in a faster reaction yield.

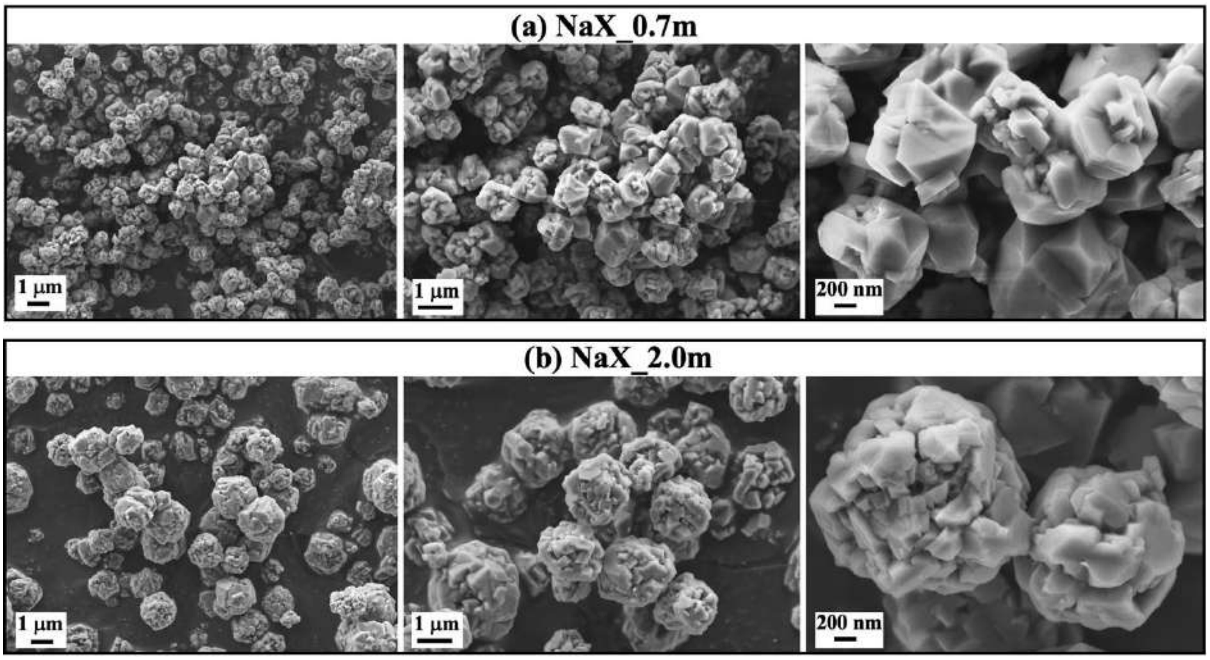

Fig. 1. SEM images of zeolite NaX with different crystal sizes.

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Posters

Thème 2
Caractérisation et Modélisation

THEME

☐ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☑ Theme 3 : Synthesis and shaping

Targeted Modification of ZSM-5 for High-Efficiency Co-Production of Para-Xylene and Light Olefins from Methanol–Toluene Co-Conversion

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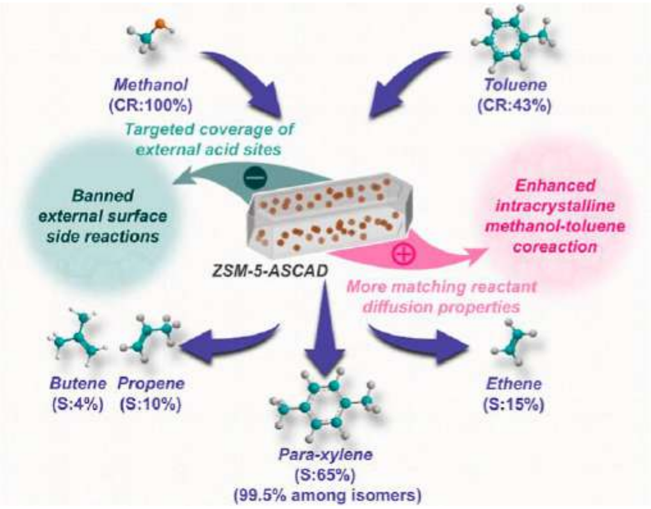
Abstract

This study presents a novel Acid Site-Chemical Adsorption–Deposition (ASCAD) method for the precise modification of ZSM-5 zeolite, achieving exceptional catalytic performance in the co-conversion of methanol and toluene. Unlike conventional Chemical Liquid Deposition (CLD), which forms a thick silica layer and severely limits diffusion, the ASCAD method employs an ultra-low concentration of tetraethyl orthosilicate (TEOS) followed by vacuum desorption to selectively deposit silica only on external acid sites while preserving intracrystalline diffusivity.

The modified ZSM-5-ASCAD catalyst exhibits outstanding shape selectivity and activity: para-xylene (PX) selectivity among xylene isomers reaches 99.5%, with a total selectivity of light olefins and PX of 94%. Importantly, toluene conversion remains high at 43%, significantly surpassing the 18% conversion observed with CLD-modified ZSM-5. Through advanced characterization techniques—including TOF-SIMS depth profiling, zero-length column diffusion measurements, infrared microscopy, and isotope labeling—we demonstrate that ASCAD minimizes non-target silica deposition, effectively suppresses external surface side reactions, and maintains matched diffusivity for both methanol and toluene.

This work introduces a targeted modification strategy that simultaneously enhances catalytic activity, shape selectivity, and carbon utilization efficiency, providing a promising pathway for the integrated production of key aromatic and olefinic chemicals from non-petroleum feedstocks.



Scheme 1. Reaction pathway change after surface modification by the ASCAD method

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Y. Wu, N. Wang, E. Chen, et al., *ACS Catal.* **2025**, 15, 5, 4147–4159

The support of the IRN China-France "Zeolites" is acknowledged.

THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Additive and Synergistic Effects in USY/ZSM-5 Systems: Role of Acidity, Composition, and Phase Intimacy in n-Hexane Cracking

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Introduction

Zeolites are stable microporous solid acid catalysts extensively used in industrial and technological applications. In industrial practice, they are commonly employed as mixtures, where combining different zeolitic phases can improve catalytic performance and selectivity through synergistic effects related to complementary pore structures and selective molecular diffusion [1]. A representative example is the incorporation of small amounts of ZSM-5 into FCC catalysts, which enhances propylene yield and increases octane number [2].

In this work, we explore the additive and synergistic effects arising from the combination of ZSM-5 and USY zeolites. To this end, mechanical mixtures with controlled composition and acidity, as well as Y/ZSM-5 composites enriched in either phase, were prepared and their catalytic behaviour was assessed using n-hexane cracking as a probe reaction for Bronsted acid site strength.

Materials and Experimental Methods

The transformation of n-hexane was carried out in a four-parallel fixed-bed reactor system. Reaction rates were evaluated at four different contact times by varying the catalyst loading. The catalyst (particle size 0.2–0.4 mm) was pre-treated at 540 °C under a nitrogen flow for 12 h. A diluted n-hexane/nitrogen mixture (molar ratio 11) was then introduced into the reactors at 540 °C.

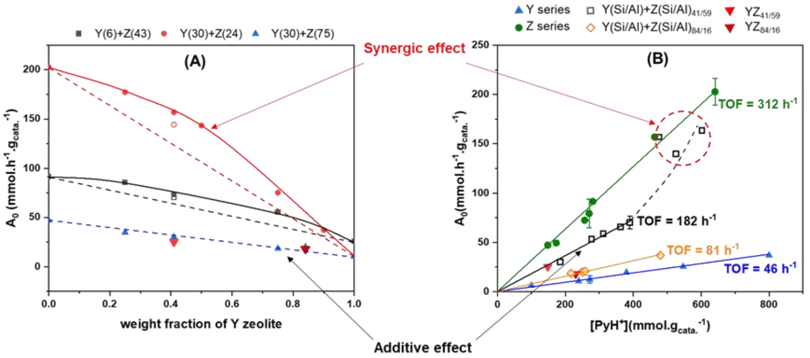

Fig. 1. Impact of phase composition (A) and concentration of Brønsted acid sites (B) on catalytic activity during n-hexane cracking at 540 °C. Dashed lines guide the eye; solid lines indicate the expected activities.

Results and discussion

Additive and synergistic effects in Y/ZSM-5 systems were investigated by varying composition, Brønsted acid site concentration, and phase intimacy. Three mixtures were studied: Y(30)+Z(24), showing strong synergy; Y(6)+Z(43), with weaker synergy; and Y(30)+Z(75), exhibiting nearly additive behaviour. As Y content increases, intrinsic activity decreases due to the higher cracking activity of ZSM-5. The composites show additive activity similar to Y(30)+Z(75), despite lower Si/Al ratios, indicating incomplete aluminium incorporation and the absence of synergistic effects.

Figure 1B shows that n-hexane cracking activity increases linearly with Brønsted acid site concentration for pure ZSM-5 and USY, indicating homogeneous and independent active sites [3]. The corresponding TOF values are 312 h^{-1} for ZSM-5 and 46 h^{-1} for USY, confirming the absence of synergistic effects. The binary systems also display a linear relationship between A_0 and [PyH$^+$], except at high acid-site concentrations for the 41/59 mechanical mixture series. In this case, the linearity cannot be ascribed to site homogeneity, as at least two populations of acid sites with different strengths are present. Overall, for both composites and intimate mechanical mixtures, the activity corresponds to the algebraic sum of the contributions from pure USY and ZSM-5. Thus, within the linear regime, the binary systems can be considered as containing two independent, homogeneous populations of acid sites.

Notably, a synergistic effect emerges at high Brønsted acid site (BAS) concentrations for the 41/59 series, particularly in mixtures containing Z(24) (Si/Al = 24). This synergy is observed across the entire composition range of Y(30)+Z(24) and also when Z(24) is combined with USY samples of different Si/Al ratios. These results indicate that a high BAS density in ZSM-5 ([PyH$^+$] = 641 μmol·g$^{-1}_{cat}$) promotes genuine synergistic interactions between ZSM-5 and USY in intimate mechanical mixtures.

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Hierarchical MOR Zeolites: Unravelling Microporosity Evolution through Organic Probe Adsorption

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Mordenite (MOR), widely employed in petrochemical catalysis for its shape-selective microporous framework, nonetheless suffers from diffusion limitations that hinder the access of bulky molecules to active sites [1]. The introduction of hierarchical porosity, particularly mesoporosity, offers an effective means of reducing diffusion path lengths and enhancing molecular accessibility. Although numerous hierarchization strategies have been reported, the actual impact of these treatments on the intrinsic microporosity of MOR remains insufficiently elucidated in the current literature [2].

In this work, we investigate how dealumination-induced porosity evolution affects the adsorption behaviour of organic probe molecules and the balance between specific interactions and steric constraints. A set of parents, commercial, and laboratory-modified MOR zeolites exhibiting a wide range of φ_{Ar} accessibility indices (0–0.76) was characterized through a multimodal approach combining n-nonane pre-adsorption, argon physisorption at 87 K, and adsorption isotherms at 298 K of molecules with increasing kinetic diameters (n-hexane, cyclohexane, 2,3-dimethylbutane, toluene) [3-4].

Micropore widening resulting from side-pockets degradation was quantitatively assessed through the φ_{Ar} index, revealing a clear relationship between dealumination severity, reduction of Brønsted acidity, and loss of confinement. Adsorption isotherms were modelled using a combined Fowler–Guggenheim/Dubinin–Radushkevich approach, allowing discrimination between specific surface interactions at low pressure and pore-filling contributions at higher loadings.

The results highlight contrasting adsorption mechanisms depending on molecular size: n-hexane and toluene adsorption remains strongly governed by Brønsted acid–base interactions and decreases with micropore enlargement, whereas bulkier molecules (cyclohexane, 2,3-dimethylbutane) exhibit enhanced uptake and higher occupation rates upon dealumination, benefitting from reduced steric hindrance in enlarged micropores. These findings demonstrate that hierarchical treatment does not uniformly improve adsorption but selectively enhances accessibility for sterically hindered molecules.

Overall, this study provides new insights into the interplay between confinement, acidity, and pore topology in hierarchical MOR zeolites, and establishes probe-molecule adsorption coupled with advanced modelling as an effective methodology for assessing microporosity evolution.

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THEME ☒ Theme 2 : Characterization and modeling

Influence of Water, NO_2, and SO_2 on CO_2 Adsorption Performance of Zeolite 13X Under Post-Combustion Conditions

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(2) Department of Chemical Engineering, Imperial College London, UK

Solid adsorbents, including zeolites, are widely studied for post-combustion carbon capture, yet their performance can be significantly affected by contaminant gases and vapours in streams. This work investigates the influence of common impurities, water vapour, nitrogen dioxide (NO_2), and sulfur dioxide (SO_2), on the CO_2 adsorption performance of zeolite 13X, a prototypical material which has shown some promise for CO_2 capture [1-2], under realistic post-combustion conditions.

We employ lab-scale (5-100mg) sorption methodologies including, gravimetric Dynamic Vapour Sorption (DVS), Breakthrough Analysis (BTA), and Temperature-Programmed Desorption (TPD), to evaluate these effects on commercially available binderless zeolite 13X beads. Confirming previous observations[3], water vapour takes precedence at equilibrium even below 1vol%, displacing CO_2 and leading to substantial reductions in CO_2 uptake. Further, NO_2 and SO_2 at trace amounts (<100ppm) exhibit strong chemisorptive interactions with the sorbent sites, causing pronounced and partially irreversible working capacity loss [4-5] of 20-60%, even after regeneration above 400°C. Our findings provide insights into the practical performance of solid sorbents in realistic operating conditions.

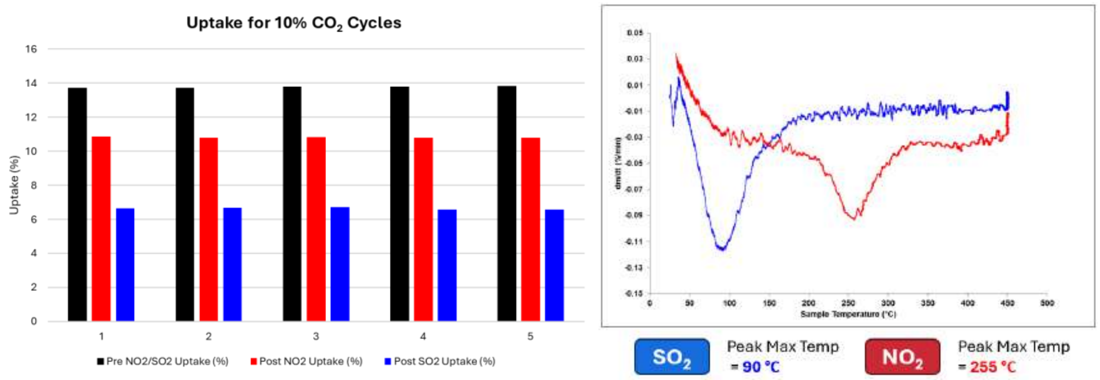

Figure 1: (Left) CO_2 Capture performance of Zeolite 13X before and after exposure to 75 ppm SO_2/NO_2. (Right) TPD experimental results showing the temperature required to desorb SO_2/NO_2.

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Mise en œuvre de l'Ag@ZM-5 dans un procédé d'adsorption modulé en température

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Dans le cadre du Traité d'Interdiction Complète des Essais nucléaires (TICE), le CEA a développé un procédé nommé le SPALAX® (Système de Prélèvement Automatique d'Air en Ligne avec analyse des radioXénons atmosphériques). Ce système suit la concentration des isotopes radioactifs du xénon afin de déceler les activités nucléaires partout dans le monde. Les radioxénons, dont les isotopes stables sont présents à hauteur de 87 ppb dans l'atmosphère, doivent être concentrés afin d'être quantifiés par la spectrométrie gamma [1].

Les études menées auparavant ont permis de montrer l'intérêt de la zéolithe ZSM-5 dopée à l'argent pour l'adsorption et la concentration du xénon – par rapport au charbon actif – notamment grâce aux sites forts dus aux nanoparticules d'argent. En revanche, l'approche expérimentale visant à expliquer la relation structure de l'adsorbant – propriétés du matériau arrivant à ses limites, un couplage expérimental et modélisation a été réalisé afin de caractériser les données thermodynamiques d'adsorption et de diffusion [2].

L'objectif général de la thèse est donc d'identifier des technologies en rupture avec celles utilisées actuellement afin de mettre l'Ag@ZSM-5 en œuvre dans les meilleures conditions possibles. Ce travail est axé sur l'exploration et le développement méthodologique en étudiant plusieurs aspects : les moyens de chauffage du matériau, la modélisation des propriétés physico-chimiques et thermodynamiques du matériau afin de seconder les expériences et aider à la détermination des conditions d'usage optimales tant en termes d'adsorption que de désorption.

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Probing Acid Site Accessibility and Molecular Diffusivity in ZSM-5 Zeolites by Time-Resolved FTIR Titration

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Abstract

Understanding the accessibility of acid sites and the internal diffusivity of reactant molecules in zeolites is essential for rationalizing their catalytic behavior in hydrocarbon conversion reactions. In this work, a comparative investigation of molecular adsorption and diffusion in two ZSM-5 samples with distinct textural and acidic properties is carried out using time-resolved in situ FTIR titration spectroscopy.

Toluene and cyclohexene were selected as complementary probe molecules due to their different molecular size and chemical nature, allowing a sensitive assessment of transport phenomena within the zeolitic framework. FTIR experiments were performed under strictly identical conditions, enabling a direct comparison of adsorption capacity, site accessibility, and diffusion-related effects. Quantitative analysis was achieved by integrating characteristic vibrational bands of the probe molecules and calculating normalized fractional coverages as a function of the introduced amount.

The FTIR titration data reveal that, while one sample exhibits a higher overall adsorption capacity consistent with its larger concentration of acid sites, the second material displays a faster spectroscopic response upon probe introduction. This behavior is observed for both aromatic and olefinic molecules and indicates more efficient internal diffusion and improved accessibility of acid sites, despite a lower total adsorption capacity. The evolution of Brønsted and Lewis acid site bands, together with probe-specific vibrational modes [1], provides insight into the interaction mechanisms and transport dynamics within the ZSM-5 channels. Overall, this work demonstrates that time-resolved FTIR titration represents a powerful and sensitive approach to decouple total adsorption capacity from diffusivity effects in zeolites. The methodology provides a spectroscopic descriptor of molecular transport and site accessibility that is directly relevant for interpreting catalytic performance in reactions involving bulky or diffusion-limited reactants.

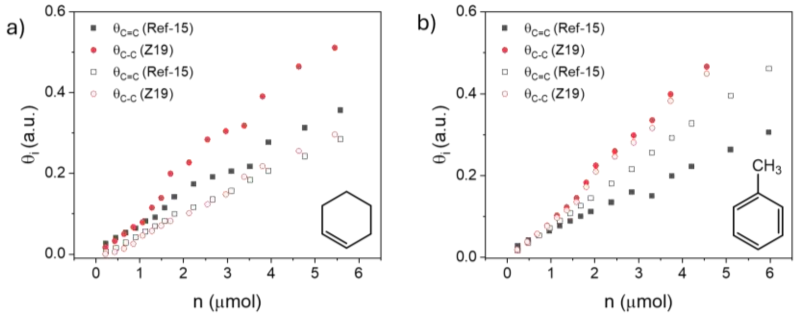

Figure 1. Evolution of the normalized fractional coverage θ_i as a function of the amount of cicloesene (a) and toluene (b) introduced, derived from FTIR titration data.

Acknowledgement: The support of the Centre for Zeolites and Nanoporous Materials, Label of Excellence, Normandy Region (CLEAR^{RN}) and the European Union (ERC, ZEOLIghT, 101054004) is acknowledged.

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THEME

☐ Theme 1 : Applications for the environment, energy, and health
☒ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

n-hexane Cracking: Understanding Exaltation By Machine Learning

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One of the most commonly used catalytic tests is n-hexane cracking, a reaction initially introduced by the Mobil company in the 1960s and still widely applied under the term "α-test" [1]. This reaction proceeds via either monomolecular or bimolecular cracking mechanisms. The rate of monomolecular cracking is particularly sensitive to the strength of Brønsted acid sites [2]. The strength of these sites is closely linked to their local environment, which includes the zeolite's structural and compositional framework, the precise location of acid sites within the framework, and the presence of extra-framework species [3]. Consequently, this catalytic test serves as a powerful tool to probe the acidic properties of zeolites.

In some cases, the presence of extra-framework aluminium species (EFALs) in the zeolite structure can lead to an enhancement of acid site strength (exaltation of the catalytic activity). This effect is well documented in the literature; however, the exact origin of this phenomenon remains a matter of debate. In this context, the application of machine learning represents a promising strategy to better understand these effects and guide the rational design of FCC catalysts with optimized acidity and performance.

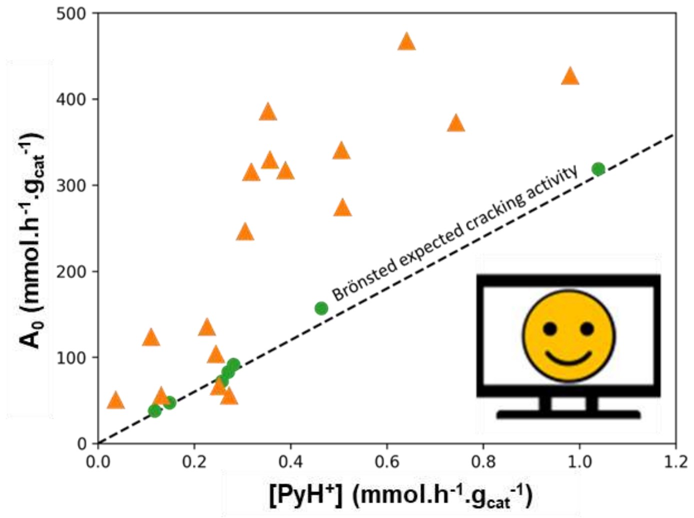

Figure 1. Plot of the catalytic activity for n-hexane cracking as a function of the Brönsted acid site density. Green circles are within 15% of the expected rate and orange triangles correspond to unexpected behaviors.

Using a machine learning model trained on a well-controlled, ZSM-5-focused in-house dataset, the catalytic activity for n-hexane cracking was investigated. The cracking activity was first categorized into exalted and non-exalted contributions. The calculated generalization error (~80 mmol.h^{-1}.g$_{cat}$$^{-1}$) demonstrates that the model successfully learned the system and highlights different activity trends as a function of Lewis and Brønsted acid site densities. By calculating the activity using the distinct trends identified, the prediction error was reduced to ~50 mmol.h^{-1}.g$_{cat}$$^{-1}$.

Furthermore, the activity-related constants (analogous to TOFs) allow the estimation of the fraction of Brønsted acid sites that are exalted, as well as the corresponding turnover frequencies of these exalted sites. Finally, the computed exalted Brønsted-to-Lewis ratios enable a discussion of the distribution of Lewis and Brønsted acid sites required to achieve site exaltation.

The results are retrospectively analyzed in terms of micro- and mesoporosity and explained by the specific characteristics of the zeolites used. Conclusions are drawn regarding the main exaltation mechanisms discussed in the literature. This seminal work breathes new life into an old model reaction and paves the way for further studies.

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Posters

Thème 3
Applications
(Environnement, énergie, santé)

THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

A multi-technique investigation of organochlorine adsorption in zeolites: linking calorimetry, TG-MS and DFT approaches

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Organochlorine compounds (OClCs), a class of persistent organic pollutants (POPs), pose serious environmental and health risks due to their toxicity, long-term stability, and bioaccumulation. They are widely used in industrial applications and are unintentionally released from waste incineration plants. The challenge is to efficiently remove these pollutants from contaminated environments. Faujasite X zeolite emerges as a good adsorbent for capturing OClCs pollutants regarding its pore opening which matches the size of the molecule, typically around 7.4 Å. This study investigates the adsorption behavior of OClCs on FAU-NaX zeolite. Adsorption experiments using isooctane as a solvent, at 298 K revealed between 3.5-4 molecules of the OClCs adsorbed per supercage of the adsorbent framework. A combined DFT prediction and microcalorimetry measurements show good agreements of the adsorption enthalpy values, varying between -80 to -132 kJ.mol^{-1}. An example of an optimized DFT adsorption configuration of 1,2-dichlorobenzene in FAU-NaX supercage is given in figure 1. The temperatures of desorption of the OClCs, which depend on the energies of interaction between the molecules and the sites of adsorption are determined by using a new method of quantification which consists of thermal gravimetric analysis (TGA) coupled to mass spectrometry analysis (MS) [1,2]. By combining infinite-dilution adsorption measurements, gas-phase enthalpy reconstruction from liquid-phase calorimetry, TG-MS desorption temperature analysis, and DFT modelling of single-molecule interactions in the FAU supercage [3], this work establishes a consistent structure-property relationship linking dipole moment, adsorption strength, and molecular-cation interaction mechanisms in FAU-NaX zeolites.

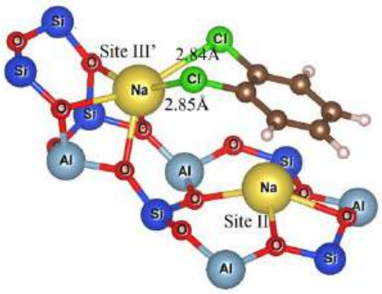

Figure 1. Optimized DFT adsorption configurations of 1,2-dichlorobenzene in FAU-NaX supercage

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THEME

☒ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Chemical Recycling of PET for MOF Synthesis

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The advancement of the Anthropocene has intensified industrial production and consumption, resulting in a continuous increase in plastic waste generation. Global plastic production has risen sharply over the past decades[1], while recycling rates remain low, with most discarded plastics being landfilled or incinerated. Among these materials, polyethylene terephthalate (PET) stands out as one of the most widely used polymers worldwide due to its extensive application in packaging, automotive, textile, and food industries, consequently representing a significant fraction of plastic waste. PET is a recyclable polymer, and chemical recycling via depolymerization has emerged as a promising strategy for its valorization[2]. Through this process, PET can be converted into valuable monomers such as terephthalic acid and ethylene glycol. Terephthalic acid, a dicarboxylic acid, is particularly relevant as an organic linker in the synthesis of metal–organic frameworks (MOFs). MOFs are crystalline porous materials composed of metal ions or clusters coordinated to organic ligands, forming two- or three-dimensional networks[3]. Due to their high surface area, tunable porosity, and structural versatility, MOFs have attracted considerable attention for applications in gas adsorption and separation, heterogeneous catalysis, and environmental remediation[4].

This work aimed to chemically recycle PET waste through depolymerization under different reaction conditions and to employ the recovered terephthalic acid in the synthesis of MOF-235 and UiO-66. MOF-235 is based on Fe^{3+} ions coordinated with terephthalic acid, while UiO-66 belongs to the UiO family and consists of Zr^{4+} clusters linked by dicarboxylate ligands. The integration of plastic waste recycling with the synthesis of high-value MOFs represents an attractive approach aligned with circular economy principles. The synthesized materials were characterized by X-ray diffraction to confirm their crystalline structure, scanning electron microscopy to evaluate morphology, thermogravimetric analysis to assess thermal stability, and nitrogen physisorption to determine textural properties. The results demonstrate that terephthalic acid can be efficiently obtained from PET under different depolymerization conditions, enabling the successful synthesis of MOF-235 and UiO-66 with structural features comparable to those reported for MOFs prepared from commercial precursors.

Overall, this study presents a sustainable pathway for PET waste valorization by coupling chemical recycling with the production of advanced porous materials, highlighting the potential of this approach for environmental catalysis and selective adsorption applications.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health
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Direct air capture of CO_2 by Ba-exchanged GIS-type zeolite

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Direct air capture (DAC) of CO_2 requires adsorbent materials capable of operating efficiently at ultra-low CO_2 partial pressures while maintaining fast kinetics and structural stability [1,2]. Zeolites are promising candidates due to their stability and tunable adsorption properties, particularly through extra-framework cation exchange. In this study, GIS-type zeolite was synthesized and systematically modified via one and three successive Ba^{2+} ion-exchange steps to tailor its framework structure and adsorption behaviour for DAC applications. PXRD analysis (Figure 1a) reveals that Ba^{2+} incorporation induces a progressive framework distortion associated with a symmetry reduction, while preserving the crystalline integrity of the GIS structure, highlighting its intrinsic structural flexibility [3].

The impact of Ba^{2+} exchange on CO_2 adsorption performance was evaluated using equilibrium adsorption isotherms and dynamic breakthrough experiments. CO_2 adsorption isotherms (Figure 1b) show that replacing Na^+ with Ba^{2+} suppresses the stepwise adsorption and hysteresis observed for Na-GIS, increases low-pressure CO_2 uptake, and enhances the saturation capacity [4]. The fully exchanged Ba3-GIS exhibits the highest DAC capacity, reaching 1.15 mmol/g at 25 °C, along with improved adsorption kinetics. These trends are further confirmed by dynamic breakthrough experiments under dry conditions (Figure 1c), where Ba3-GIS shows longer breakthrough times and higher CO_2 uptake than the partially exchanged Ba1-GIS and Na-GIS, in good agreement with equilibrium measurements.

Overall, this work demonstrates that divalent cation engineering is an effective strategy to balance adsorption strength, pore accessibility, and kinetics in small-pore zeolites, providing valuable insights for the design of robust physisorbents for atmospheric CO_2 capture.

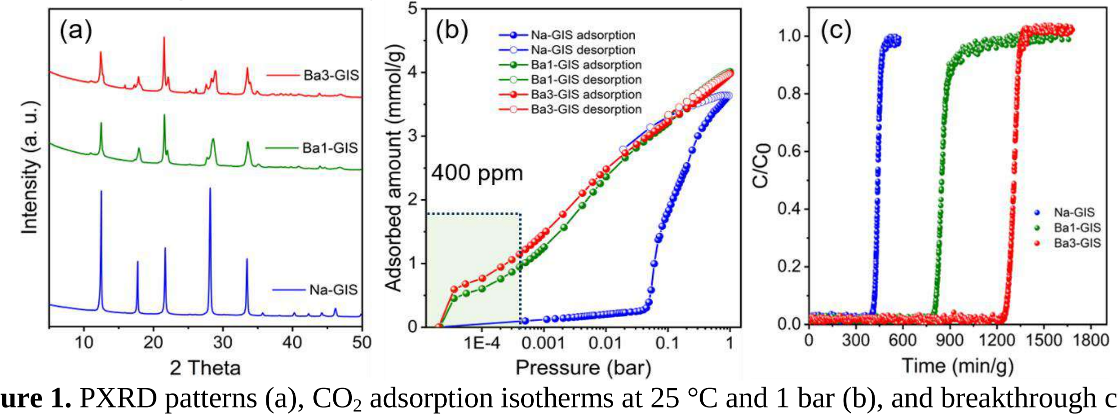

Figure 1. PXRD patterns (a), CO_2 adsorption isotherms at 25 °C and 1 bar (b), and breakthrough curve analysis under dry DAC conditions (c) of Na-, Ba1-, and Ba3-GIS.

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THEME

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☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Silanol Removal Enhances VOC Adsorption in Mo-MFI Zeolites: An Experimental–Computational Approach

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Abstract

Efficient systems to control and reduce the emissions of VOCs in general and acetone in particular is an essential challenge for society.[1,2] An efficient adsorption of acetone strongly depends on the hydrophobicity of the zeolite surface. Here, the competitive adsorption of acetone and water vapor onto pure silica MFI and molybdenum-modified MFI zeolites were examined using force field Monte Carlo and density-functional theory calculations, in situ FTIR, and Breakthrough analysis. Simulations reveal that in pure silica MFI, acetone interacts with vicinal silanol groups and silanol nests, where polar Si–OH groups dominate the adsorption process. Incorporation of molybdenum effectively anneals these silanols, generating a significantly more hydrophobic framework in which acetone adsorption is driven primarily by coordination of the carbonyl oxygen to metal sites. In situ FTIR measurements confirm extensive hydrogen bonding of acetone to germinal, isolated, and nest silanols in pure silica MFI, while Mo-containing MFI largely devoid of surface silanols promoting predominantly physisorption within the straight channels. Breakthrough studies confirm the enhanced adsorption acetone selectivity, even in the presence of water vapor. Together, experiments and simulations demonstrate that Mo-containing, silanol-annealed MFI zeolites are highly efficient microporous adsorbents for selective acetone/water separation and acetone detection.

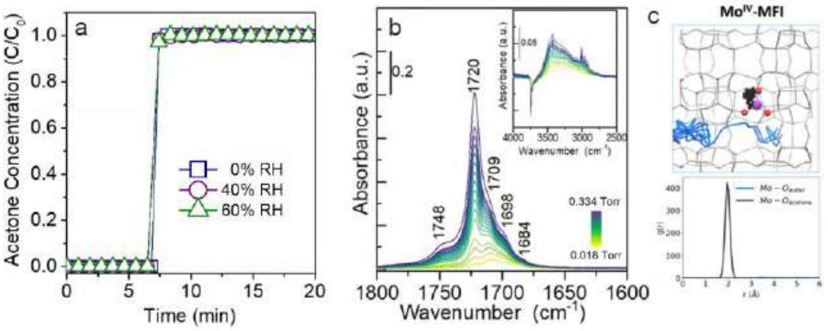

Fig. 1. (a) Breakthrough curves of acetone at different relative humidity for Mo-MFI, (b) FTIR spectra of acetone adsorbed on Mo-MFI, under increase acetone doses and (c) Simulations trajectory and associated radial distribution function for acetone/water and MFI atom pairs.

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Sustainable Synthesis of Analcime Zeolite from Natural Silica and Coal Fly Ash: Taguchi Optimization and Adsorption Performance

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Abstract

Zeolites are currently of significant importance as nanomaterials in selective adsorption, ion exchange, and heterogeneous catalysis. However, the limited availability and rising cost of conventional precursors, combined with zeolites increasing global demand, underscore the need to explore low-cost, abundant alternative raw materials. This study focuses on the zeolitization of natural silica and coal fly ash by-product through an innovative approach using the L9 Taguchi orthogonal array to optimize key synthesis parameters, namely NaOH concentration, synthesis duration, hydrothermal temperature, and the SiO_2/Al_2O_3 mass ratio. The resulting powders were characterized using various analytical techniques, including XRD, FTIR, SEM/EDX, and DTA/TG. The zeolitization rate of the starting materials was considered the response parameter, and the influence of operational factors was assessed using ANOM /ANOVA analyses. Under optimal conditions (160 °C, 36 h, 1.5 M NaOH, and SiO_2/Al_2O_3 mass ratio of 2.2), a zeolitization efficiency of 89% was achieved, with analcime identified as the dominant crystalline phase. Subsequently, the adsorption performance of the optimal sample was evaluated using methylene blue (MB) as a model contaminant. Kinetic studies indicated that the adsorption followed a pseudo-second-order model, suggesting chemisorption as the dominant mechanism. Equilibrium data fit well with the Langmuir, Freundlich, and Temkin isotherm models, indicating that the adsorption involves both monolayer coverage and heterogeneous surface interactions. Under optimal conditions (MB 40 mg L^{-1}, pH 12, contact time 80 min, adsorbent dosage 2 g L^{-1}), a high removal efficiency of 99.69% was achieved, confirming the effectiveness and cost-efficiency of the synthesized analcime zeolite.

Reference

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Efficiency of MOFs, Zeolites, and Activated Carbon as VOC Shields in Pharmaceutical Packaging

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Molecular pollution management has become a critical challenge across pharmaceutical industries. Volatile organic compounds (VOCs) can be released during extrusion and injection processes, degassing of packaging materials, or polymer aging. Common VOCs such as limonene, tetrahydrofuran (THF), benzaldehyde, and formaldehyde are frequently present as impurities in polymers or generated *in situ* through polymer degradation. Their release within packaging environments can negatively impact drug stability through interactions with active pharmaceutical ingredients (APIs), or degradation pathways, while also posing risks to patient safety (nitrosamine formation in the case of formaldehyde).

In this study, seven porous adsorbents including MOFs (MOF A520(Al), MOF-801(Zr), CAU-10(Al)-H, ZIF-8(Zn)), zeolites (**MFI**, **FAU**), and activated carbon were evaluated for their ability to trap VOCs under controlled conditions. Breakthrough experiments with gaseous formaldehyde (2 ppm, 23 °C, dry air) show superior performance of hydrophilic adsorbents, like zeolite 13X adsorbing 41.28 mg/g. At 50% relative humidity, adsorption capacity decreases sharply for all hydrophilic materials, with activated carbon showing the best performance. For THF (Figure 1), kinetic experiments realized at 25 °C and $p/p^0 = 0.5$, ZIF-8(Zn), and MOF-801(Zr) challenge activated carbon (with uptakes of 344.3, 294.5 and 354.7 mg/g, respectively). Limonene adsorption is most effective with activated carbon and MOF-801(Zr) (346.6 and 297.9 mg/g). Benzaldehyde scavenging at 20 °C under saturated pressure, shows best results with activated carbon, ZIF-8(Zn), and MOF-801(Zr) reaching 461.8, 452.5, and 402.7 mg/g, respectively. These results highlight the potential of porous materials to mitigate VOC contamination in pharmaceutical packaging, ensuring improved drug stability and patient safety.

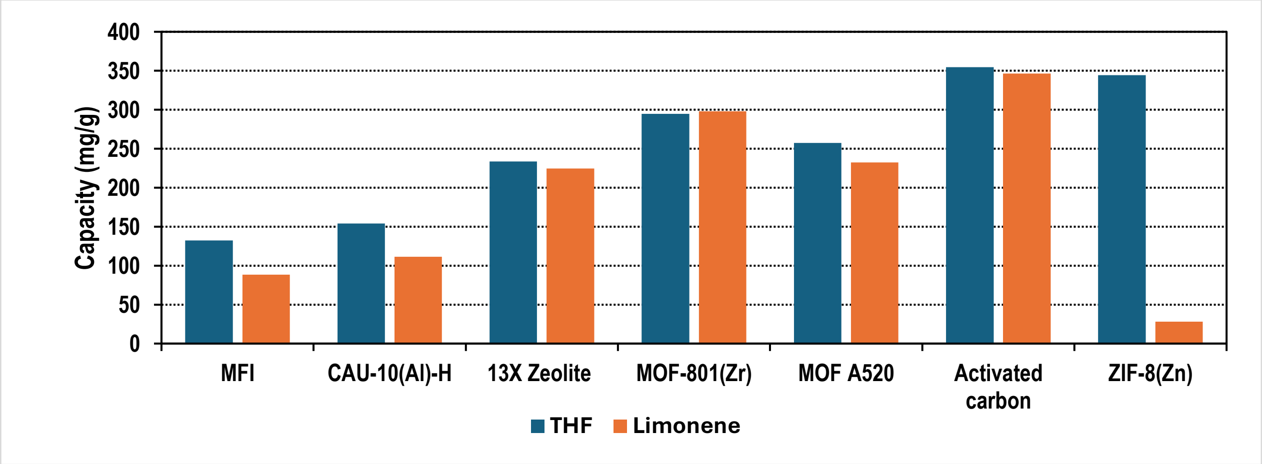

Fig. 1. Representation of the scavenging capacities of seven porous materials towards THF and limonene at 25°C and $p/p^0 = 0.5$)

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Low-Spin-State Fe^{III}-Layered Double Oxide/Zeolite-P1 Nanocomposite Tuned for Pollutant Adsorption in Simulated Wastewater: DFT-Guided Mechanistic Insights and BBD-Improved Batch to Column Transferability

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Abstract

For the first time, a Zeolite-P2 seed-assisted hydrothermal treatment is reported that synthesizes low-spin-state Fe^{III}-LDO/Zeolite-P1. In terms of cost, this synthetic nanocomposite with 311.19 m^2 g^{-1} surface area amounts to ~0.68 USD per gram.

To assess its efficiently, we proposed the sorption of two typical azo dyes with different polarities, Congo red (CR) and methylene blue (MB). Furthermore, we systematically investigated the batch-to-column transferability, which was improved through the Box Behnken Design (BBD) statistical analysis.

In batch experiments, the results demonstrated that the pseudo-second-order (PSO) was in harmony with our sorption data, with removal efficiencies of 96.4% for CR (pH 5) and 92.1% for MB (pH 9) at 5 mg·L^{-1} after 210 min. Importantly, the strong host-guest chemisorption is dominates the mechanism. This was clarified at the atomic level via density functional theory (DFT). DFT revealed that the interaction involving Fe^{III}-O-Si (electron transfer LDO-to-Zeolite) facilitated the uptake of CR by the low spin Fe^{III} sites, and thereby shows superior electrostatic multilayer adsorption performance; this observation was supported by the shortened Fe^{III}-O bond length from 2.138 Å (high spin) to 1.819 Å (low spin) and increased d-band center from −2.93 eV to −1.96 eV in the presence of the CR molecules, consistent with the X-ray photoelectron spectroscopy (XPS) results.

For batch-to-column transferability, breakthrough time (BT) was identified as a function of its key influential factors: capacity (q_e) and kinetics (k_2) fitted with PSO. A notable enhancement in q_e and k_2 was spotted after BBD analysis, with a desirability of 1.00, achieving >92% accuracy in BT estimation. With reuse over 3 cycles for CR and 5 cycles for MB, the cost of removing 1 g of dye from simulated wastewater is ~9.88 USD and ~11.70 USD, respevtively.

Finally, this study provides insights that may guide both future catalytic conversion of oxygen-containing molecules.

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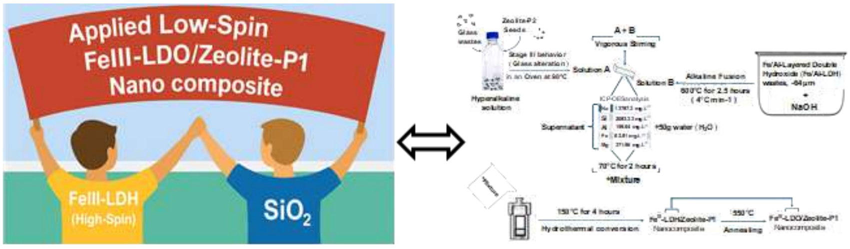

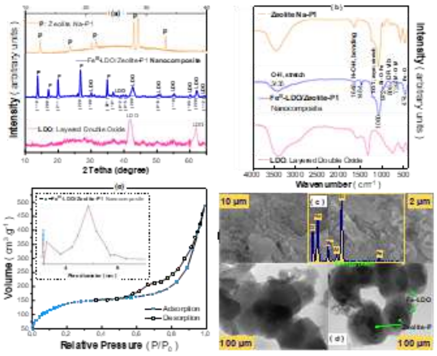

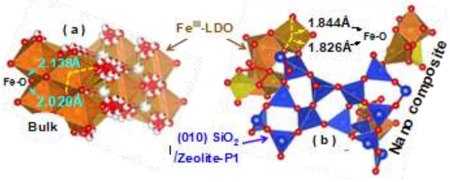

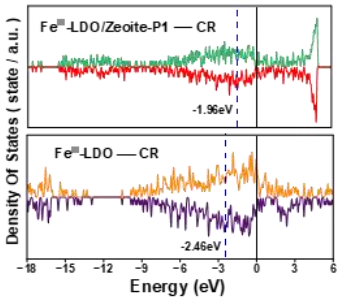

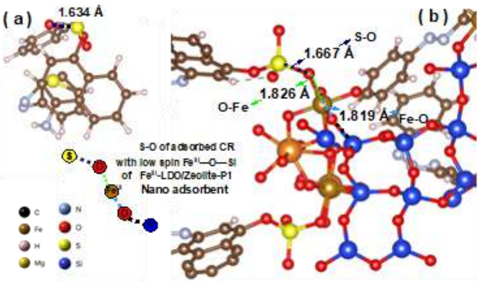

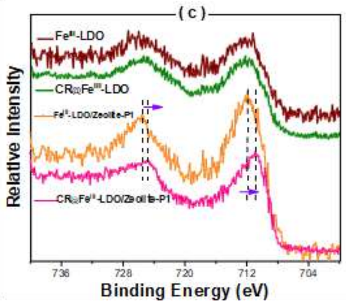

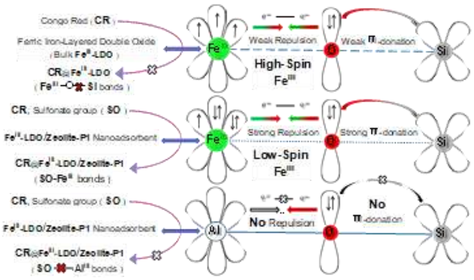

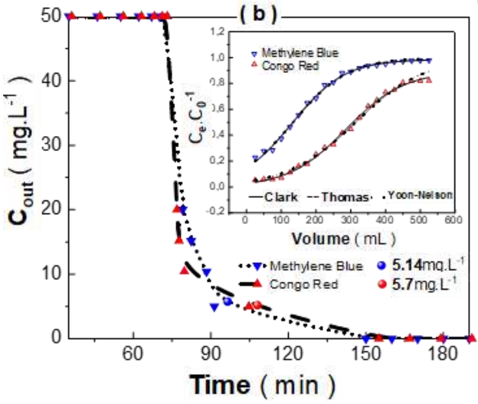

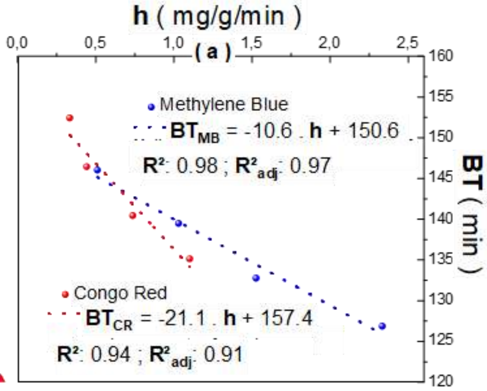

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THEME

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Effect of Ni, Mo, and W on Oleic Acid Hydroconversion Pathways over Nano-ZSM-5 Catalysts

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The aviation sector plays a central role in modern society, yet it remains one of the most difficult sectors to decarbonise. Consequently, sustainable aviation fuels derived from renewable resources are attracting increasing attention as viable alternatives to conventional jet fuels [1]. In this work, oleic acid was selected as a representative model compound to investigate the catalytic hydroconversion of fatty acids into aviation-range hydrocarbons (C8–C15) through an integrated reaction network involving hydrodeoxygenation, hydrogenation, isomerisation, cracking, and aromatisation. A series of catalysts consisting of 5 wt% Ni, Mo, and W supported on nano-sized ZSM-5 zeolite was evaluated under identical reaction conditions (20 bar H_2, 300 °C, 6 h). In all cases, oleic acid conversions exceeded 90%, indicating high activity irrespective of the supported metal. However, despite similar conversion levels, pronounced differences were observed in product distribution. For bare n-ZSM-5 and the Mo- and W-supported catalysts, high conversion mainly led to heavy products that, although detectable by GC–MS, could not be reliably identified, leaving a significant fraction of the product slate chemically undefined. In contrast, the introduction of Ni profoundly altered the hydroconversion pathway. Over Ni/n-ZSM-5, no unidentified heavy products were observed, and the entire heavy fraction could be confidently assigned by GC–MS. This fraction is dominated by long-chain hydrocarbons, with heptadecane and octadecane as the main products, evidencing efficient hydrodeoxygenation and suppression of uncontrolled condensation pathways. Water and CO_2 were identified as the main oxygen removal products, while CO was detected only in trace amounts, indicating a preference for hydrodeoxygenation and decarboxylation over decarbonylation. In addition, Ni/n-ZSM-5 promotes the formation of an aviation-range fraction rich in aromatics, which accounts for approximately 70 wt% of the hydrocarbon products. Despite the successful production of aviation-range hydrocarbons, the resulting jet fuel fraction does not meet current fuel specifications due to an overly high aromatic content. Therefore, while Ni is essential to obtain a chemically well-defined product slate, further catalyst optimisation is required to balance cracking, aromatisation, and isomerisation reactions. Future efforts will focus on tailoring the zeolite support by moderating acidity and improving pore accessibility. In this context, dendritic zeolite architectures represent a promising strategy to better control secondary reactions and move toward SAF compositions compliant with regulatory requirements.

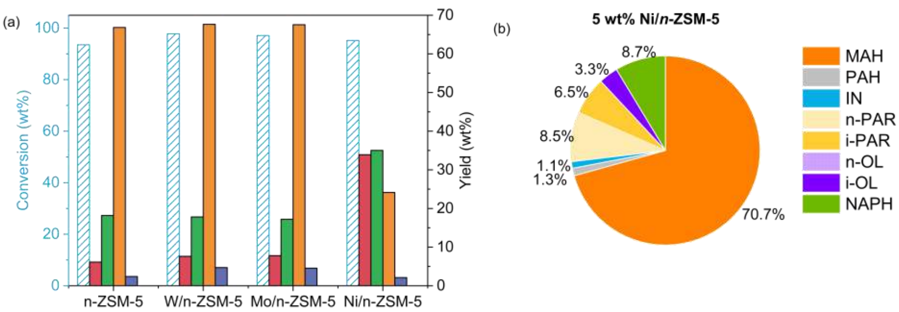

Fig. 1. Results of oleic acid hydroconversion: (a) conversion and yields, and (b) molecular composition of jet fuel fraction (C8-C15). MAH: mono-aromatics, PAH: poly-aromatics, IN: indanes, PAR: paraffins, OL: olefins and NAPH: naphthenes.

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Influence of Si/Al ratio and cation types in the synthesis of glycerol carbonate from glycerol and dimethyl carbonate

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Glycerol (Gl) is a byproduct of biodiesel production, but it has low value as a chemical. The aim of this work is to transform glycerol into a value-added product, glycerol carbonate (GLC). Pan et al. [1] compared the performance of Na-based zeolites, including Beta, LTA, ZSM-5, and NaY in the synthesis of GLC from GL and dimethyl carbonate (DMC). NaY zeolite exhibits high yield, selectivity, and stability. Recently, Kosawatthanakun et al. [2] increased the basicity of BPH zeolite by exchanging the cation to Na^+ , K^+ , and Cs^+ forms. From the literature, to increase the basicity by changing NaY to NaX, which has a high sodium cation and basicity. Moreover, the cation types of zeolite Y and X in Na and K forms were compared. The zeolites were synthesized by hydrothermal method using a silica source from silica gel waste. The catalysts were characterized using XRD, SEM, FTIR, BET, and N_2 analysis. The zeolite basicity increases after exchange to K cation (Figure 1a). The GLC conversion, selectivity, and yield were analyzed by HPLC/RID. The influence of zeolite cation types, both NaX and NaY, gives a better performance than the KX and KY (Figure 1b). NaX zeolite gives a higher GLC yield (96%) than NaY (92%) from a 3 h reaction time and selectivity close to 100%.

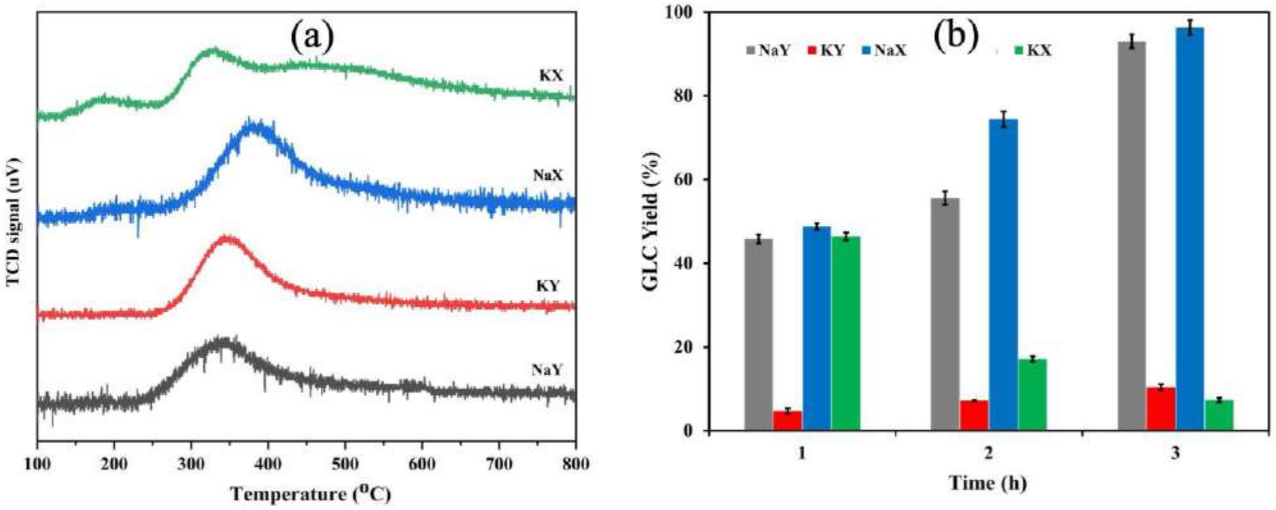

Fig. 1. (a) CO_2-TPD profiles of zeolite Y and X in Na and K form and (b) GLC yield of zeolite Y and X in Na and K form at various times.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

Utilisation des zéolithes pour préserver les propriétés organoleptiques des vins

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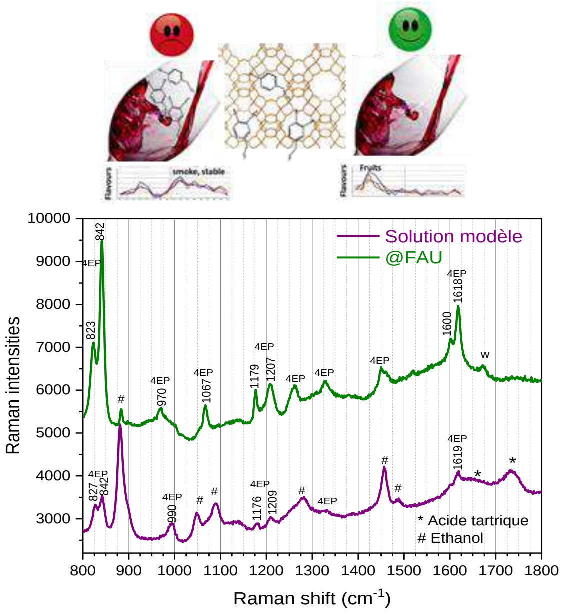
Dans les vins, la présence de certains composés peut entraîner des déviations organoleptiques et sensorielles préjudiciables. Ces composés peuvent par exemple résulter de la présence de levures d'altération dans les vins ou de l'oxydation de certains produits de fermentation. Ces molécules peuvent parfois être perçues à des concentrations extrêmement faibles (quelques µg/L) et conduire à des déclassements de lots de vin. Les techniques d'élimination de ces composés autorisées par l'OIV (filtration membranaire, utilisation de charbons actifs) peuvent s'avérer couteuses, difficiles à mettre en place dans une exploitation viticole et/ou peu sélectives.

Dans ce travail, différentes zéolithes ont été évaluées lors d'expérimentations d'adsorption de quatre composés (4-éthylphénol (4EP), 4-éthylgaïacol (4-EG), sotolon (SOT) et aminoacétophénone (AAP)) conduites en mode batch à partir de solutions hydroalcooliques représentatives de vins. Les résultats montrent que les cinétiques d'adsorption sont rapides pour les quatre composés et que les isothermes peuvent être décrites par un modèle de Langmuir. Cependant, de fortes disparités sont observées au niveau des sélectivités liées à la chimie du milieu. Dans le cas des phénols volatils, les résultats montrent qu'un choix approprié de l'adsorbant permet de réduire significativement les effets de compétition liés à la présence d'eau, d'éthanol et d'acide tartrique (figure 1). Néanmoins, ce choix s'avère délicat quand la solubilité des molécules indésirables est forte ou que leur pKa est proche du pH du vin (SOT et AAP, figure 2).



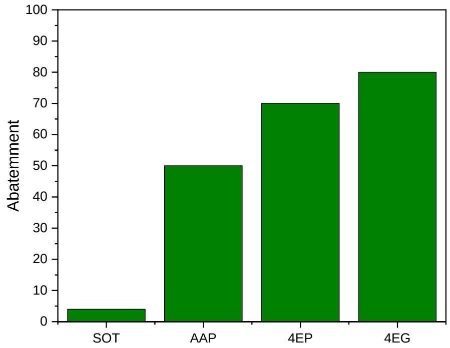


Figure 1 : Spectres Raman de la phase adsorbée 4EP sur zéolithe FAU en solution hydroalcoolique et propriétés organoleptiques des vins avant et après adsorption du 4EP

Figure 2 : Taux d'abattement du SOT, AAP, 4EP et 4EG dans les solutions hydroalcooliques après adsorption sur la zéolithe FAU

THEME

☑ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

Enhancing catalytic performance of potassium supported on zeolite NaY prepared by potassium formate buffer for transesterification of glyceryl trioctanoate

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Zeolite-based solid base catalysts offer a promising pathway toward sustainable biodiesel production, yet their practical application is often limited by framework collapse during alkali metal incorporation[1,2]. In this work, we demonstrate a strategy to preserve zeolite NaY crystallinity while enhancing catalytic performance by employing a potassium formate buffer (HCOOH/HCOOK) as a mild precursor for potassium introduction. Calcination at only 400 °C enables the controlled in situ formation of highly dispersed K_2CO_3 within the NaY framework, while significantly suppressing zeolite collapse compared to conventional acetate-derived systems. Comprehensive characterization reveals improved textural properties, stronger basicity, and superior dispersion of active carbonate species arising from the reduced hydrothermal stress and smaller precursor size. Consequently, the optimized 12K-F/NaY catalyst achieves up to 89.2% yield of methyl octanoate from glyceryl trioctanoate, surpassing potassium acetate analogues by approximately 10%. These findings highlight the critical role of precursor chemistry in tailoring zeolite stability and catalytic functionality, providing valuable insights for the rational design of zeolite-based base catalysts.

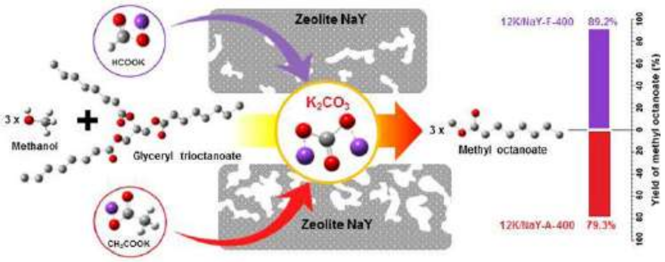

Fig. 1 Enhancement of transesterification activity over potassium-supported zeolite NaY prepared via a potassium formate buffer route.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Influence de la température et de la nature du cation sur l'adsorption de CO_2 par les zéolithes X et Y

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Les émissions de dioxyde de carbone (CO_2) jouent un rôle crucial dans le réchauffement planétaire, rendant ainsi les efforts de décarbonation et de limitation du rejet des gaz à effet de serre primordiaux pour l'industrie. Dans ce contexte, la captation de CO_2 en phase gazeuse pour le stocker et/ou le valoriser est un domaine de recherche en constante expansion. L'adsorption de CO_2 à grande échelle par les matériaux poreux constitue un procédé émergeant et alternatif au lavage par les amines, la technologie actuellement la plus utilisée [1]. Les zéolithes sont largement explorées en tant qu'adsorbants de CO_2 grâce à leur structure cristalline microporeuse et leur forte capacité d'adsorption [2]. Cependant, la très grande majorité des études se limite à des températures proches de l'ambiante alors que les températures intermédiaires (100 - 200 °C) reflètent davantage les conditions thermiques des fumées de combustion (refroidies) qui représentent une source majeure des émissions industrielles de CO_2.

Dans le cadre de ce travail, des tests d'adsorption de CO_2 par suivi gravimétrique sur des zéolithes de type structural **FAU** (faujasite X et Y) à des températures de 100 et 120 °C ont été réalisés. L'influence de la nature du cation de compensation (Na^+, K^+, Ca^{2+}, Ba^{2+}) et de leur teneur (rapport Si/Al) a été étudiée. Ainsi quelle que soit la zéolithe, la capacité d'adsorption de CO_2 augmente avec la diminution de la température. Les zéolithes X montrent des capacités d'adsorption largement supérieures à celles des zéolithes Y grâce à une densité de sites cationiques plus élevée. La nature du cation impacte également l'adsorption de CO_2. Les meilleurs résultats ont été obtenus avec les zéolithes échangées au baryum, où la capacité d'adsorption atteint 1,88 mmol/g à 100 °C et 1,30 mmol/g à 120 °C (8,3 et 5,9 % massique de CO_2, respectivement). La capacité d'adsorption varie dans l'ordre : BaX > CaX > NaX ≈ KX à 120°C et BaX > NaX > KX > CaX à 100 °C. Cette étude montre également que le protocole de régénération, basé sur un balayage sous azote à la même température que celle de l'adsorption, est efficace pour toutes les zéolithes, à l'exception de CaX et CaY.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health

☐ Theme 2 : Characterization and modeling

☐ Theme 3 : Synthesis and shaping

L'influence drastique de la nature du cation sur l'intrusion-extrusion de solutions salines dans la zéolithe hydrophobe de type FAU

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Les zéolithes à caractère hydrophobe (fort rapport Si/Al ou purement siliciques (zéosils)) présentent un grand intérêt pour les applications dans le domaine de l'absorption et du stockage d'énergie mécanique par intrusion-extrusion sous haute pression d'eau et de solutions salines aqueuses. L'utilisation de solutions salines concentrées permet d'augmenter considérablement les performances énergétiques de ces systèmes [1] en raison des phénomènes osmotiques ainsi que des énergies mises en jeu lors de la distorsion et de la déshydratation des ions solvatés durant l'intrusion. Dans le cas de systèmes « zéosil de type **MFI** – solution saline », il a été montré que la nature des ions de ces solutions salines a une forte influence sur le comportement énergétique et la pression d'intrusion [2,3]. L'étude de l'intrusion de solutions salines dans d'autres zéolithes hydrophobes présente un grand intérêt pour mieux comprendre le phénomène. La zéolithe de type structural **FAU** (faujasite) à fort rapport Si/Al (caractère hydrophobe) dont l'ouverture de cages à 12 atomes Si ou Al mesure 0,74 nm et dont le diamètre des cages est de 1,1 nm apparait comme une bonne candidate pour étudier l'influence de la nature du cation sur l'intrusion-extrusion de solutions salines.

L'intrusion-extrusion de solutions aqueuses de chlorures de métaux alcalins et alcalino-terreux (Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}), avec divers rapports molaires H_2O/sel, dans la faujasite à un rapport Si/Al = 385, a ainsi été étudiée. Contrairement au zéosil de type **MFI** [3], la nature du cation est très fortement impactant sur le comportement des systèmes « faujasite – solution saline ». Lors de l'intrusion des solutions ayant un rapport molaire H_2O/sel = 12, le système « faujasite – solution de LiCl » montre une combinaison de comportements de type amortisseur et pare-chocs pour le premier cycle d'intrusion-extrusion et un comportement amortisseur pour les cycles suivants. Par ailleurs, l'intrusion des solutions de KCl et de $MgCl_2$ est associée à un phénomène irréversible et à un comportement de type pare-chocs. L'intrusion des solutions de NaCl et de $CaCl_2$ est, quant à elle, totalement réversible, mais diffère dans le comportement du système correspondant. Le système « faujasite – solution de NaCl » montre un comportement de type ressort, tandis que le comportement de type amortisseur est observé pour la solution de $CaCl_2$. De plus, la pression d'intrusion varie fortement de 4,5 à 29 MPa en fonction de la nature du cation et de la concentration des solutions salines. Contrairement au zéosil de type **MFI** [3], la pression d'intrusion dans le cas de la faujasite, n'est pas directement liée à la taille et la charge du cation. Une forte influence de la concentration de sels sur le comportement et la pression d'intrusion est néanmoins observée.

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THEME

☒ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Pérovskites à base de halogénures de bismuth encapsulées dans des silices mésoporeuses pour la photoréduction de CO_2

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Récemment, les pérovskites halogénées de formule générale ABX_3 ou $A_3B_2X_9$ ($A = Cs^+$, $CH_3NH_3^+$… ; $B = Pb^{2+}$, Sn^{2+}, Bi^{3+}; $X = I^-$, Br^- ou Cl^-), se sont imposées comme une classe de matériaux prometteuse pour l'optoélectronique grâce à leur haute efficacité, leur faible coût et leur facilité de fabrication. Leurs coefficients d'absorption élevés, leurs bandes interdites appropriées, la dissociation spontanée des excitons et leur grande immunité aux défauts en font des matériaux très prometteurs pour diverses applications optoélectroniques ainsi que pour la photocatalyse. Les pérovskites de taille nanométrique présentent des performances photocatalytiques améliorées grâce à leur grande surface active, leur bande interdite dépendant de leur taille et leur mobilité accrue des porteurs de charge. Afin d'exploiter pleinement le potentiel des pérovskites halogénées sans plomb en tant que photocatalyseurs, les matériaux à base de nanocristaux encapsulés dans les matrices poreuses peuvent être développés. Les pérovskites halogénées sans plomb présentent un intérêt particulier grâce à leur faible toxicité.

Dans ce travail, nous présentons la synthèse de nouveaux nanocomposites à base de pérovskites halogénées de bismuth encapsulées dans des matrices de silices mésoporeuses organisées. Les silices mésoporeuses de type MCM-41 et SBA-15 ayant des mésopores unidimensionnels avec une taille de 2,4 à 8,9 nm ont été synthétisées via le procédé d'autoassemblage coopératif en présence de tensioactifs. Les nanocristaux $Cs_3Bi_2X_9$ (où $X = Br^-$ ou I^-) ont été obtenus à l'intérieur de leurs pores par imprégnation simultanée des halogénures correspondants à partir de solutions organiques. Les nanocomposites ont été caractérisés par différentes méthodes physicochimiques, structurales et texturales, leurs propriétés optiques ont été étudiées. Ils ont été testés comme catalyseurs pour la photoréduction de CO_2. Les nanocristaux encapsulés montrent une activité photocatalytique très élevée et une bonne sélectivité envers les hydrocarbures.

THEME

☒ Theme 1 : Applications for the environment, energy, and health
☐ Theme 2 : Characterization and modeling
☐ Theme 3 : Synthesis and shaping

Zeolites for SAF: From structure-property relationship to Catalyst performances

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Aviation contributes nearly 2.4% of global CO_2 emissions, making the rapid deployment of effective decarbonization strategies imperative[1]. Sustainable Aviation Fuels (SAF), produced from renewable feedstocks and fully compatible with existing jet fuel standards, represent a promising solution, with potential greenhouse gas emission reductions of 50–80%. However, their large-scale deployment remains constrained by high production costs and limitations in catalytic efficiency, identifying catalyst design as a key technological bottleneck.

Several SAF production pathways have been certified under ASTM D7566. Among them, the HH-SPK route (Hydroprocessed Hydrocarbons from Algae, certified in 2020) enables the valorization of microalgal biomass such as *Botryococcus braunii*.[2] In this pathway, the final upgrading step, hydroisomerization, is critical to fuel quality, as it converts long-chain linear alkanes into branched paraffins (C_9–C_{14}) with the cold-flow and combustion properties required for aviation fuels[3].

Hydroisomerization is a bifunctional catalytic process in which the acidic, structural, and diffusion properties of the zeolitic support govern activity and selectivity toward isoparaffins. Accordingly, this study adopts a structure-driven approach centered on zeolite framework design. To enable meaningful comparisons, the metallic function is standardized using platinum with optimized loading, ensuring well-balanced bifunctional catalysts under clean-feed conditions, where hydrogenation–dehydrogenation and isomerization rates are properly matched.

The zeolites investigated were selected to span a broad and rational range of pore sizes and topologies, allowing the systematic assessment of confinement and diffusion effects in hydroisomerization. **Medium-pore** ZSM-22 (1D, 10-MR, ~5.5 Å) represents strongly confining environments, while **large-pore** Beta and USY zeolites (3D, 12-MR, ~6.6–7.4 Å) provide increased accessibility with differing acidity and connectivity. These references are compared to **extra-large-pore** frameworks, including **UTD-1** (14-MR, ~8.5–9 Å), **ZEO-1** (3D, 12–16 MR, ~11.9 Å) and **ZMQ-1** (3D, 28-MR, ~22.8 Å), which offer reduced diffusion limitations while retaining zeolitic acidity. Their catalytic performances in dodecane hydroisomerization under 20 bar are systematically benchmarked (Fig. 1) to elucidate how pore architecture, acid site distribution, and transport phenomena control activity, and selectivity. ZSM-22 exhibits high C12 isomer selectivity due to its narrow 1D pore system, which imposes strong steric confinement that favors skeletal isomerization while suppressing β-scission. In contrast, 3D large-pore zeolites such as Beta and USY reduce shape selectivity and promote secondary reactions, leading to increased cracking. Extra-large-pore 3D frameworks (UTD-1, ZEO-1, ZMQ-1) provide insufficient confinement, resulting in dominant cracking pathways and low C12 isomer yields.

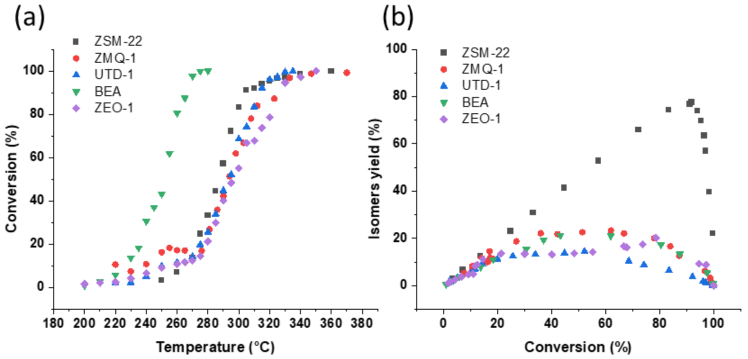

Fig. 1. (a) Conversion versus temperature and (b) isomer yield versus conversion over different Pt/zeolite catalysts under identical reaction conditions.

Overall, this study establishes robust **structure–property relationships** for zeolite-based hydroisomerization catalysts, providing key insights for the rational design of advanced catalytic materials tailored to sustainable aviation fuel production.

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Assemblée générale

Jeudi 2 avril 2026 à 10h00

A l'issue du renouvellement des membres du Comité du GFZ par l'Assemblée Générale de l'association qui s'est tenue le 03 avril 2025, le nombre de personnes siégeant au Comité du GFZ était de 9, conformément aux statuts de l'association.

Composition du comité :
- Carmen Ciotonea (Trésorière), UCEIV - Dunkerque
- Bogdan Harbuzaru (Secrétaire), IFPEN - Solaize
- Emily Bloch (Présidente), Madirel - Marseille
- Alexandre Legrand (Membre, Webmaster), UCCS - Lille
- Rémy Guillet-Nicolas (Membre) LCS - Caen
- Louwanda Lakiss (Membre), LCS - Caen
- Eddy Dib (Membre), LCS - Caen
- Andrey Ryzhikov (Membre), IS2M - Mulhouse
- Julien Grand (Membre), TotalEnergies - Feluy

Représentant doctorant (e) / post-doctorant (e) :
- Julia Duplessis-Kergomard, Madirel - Marseille

L'assemblée devra procéder au remplacement ou renouvellement de trois membres du comité et au remplacement du Représentant doctorant (e) / post-doctorant (e)
- Alexandre Legrand (Membre, Webmaster), UCCS - Lille (fin 1er mandat)
- Rémy Guillet-Nicolas (Membre) LCS - Caen (fin 1er mandat)
- Andrey Ryzhikov (Membre), IS2M - Mulhouse (fin 1er mandat)

Pour pourvoir au remplacement de ces membres sortants, le comité recevra les candidatures lors de la réunion du GFZ. Ces candidatures seront soumises au vote lors de l'Assemblée Générale. Les candidats sont priés de se faire connaître auprès d'un membre du bureau avant le mercredi 01 avril, 18 heures.

Groupe Français des Zéolithes
GFZ

GFZ 2026

$41^{ème}$ réunion annuelle

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