Approches computationnelles des matériaux hybrides poreux et membranes pour un captage efficace du CO_2

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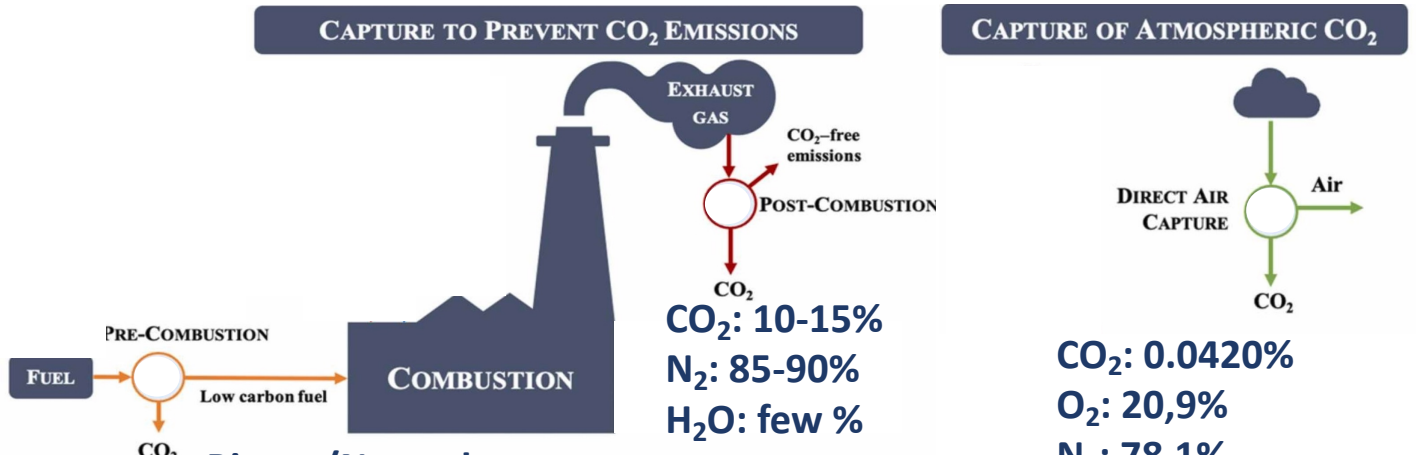
CHEMISTRY: MOLECULES TO MATERIALS

5ème rencontre académie-industrie du CNC
CO_2 déchet ou matière première: Etat de l'art et Perspectives
4 Décembre 2025, Maison de la Chimie

CO_2 capture

Different scenarios



CO_2: 10-15%
N_2: 85-90%
H_2O: few %

Biogas/Natural gas
CO_2: 40-50%
CH_4 : 50-60%

CO_2: 0.0420%
O_2: 20,9%
N_2: 78,1%
H_2O: various RH

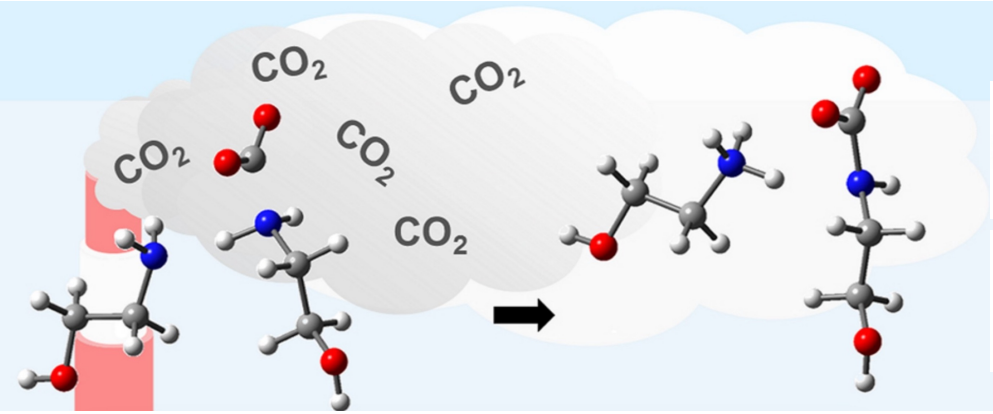
Alternative capture solution

Advanced Porous Materials

→ Adsorbent (Physisorption)-processes

→ Membrane-technologies

Current strategy: Alkanol-Amine Liquid Solvent

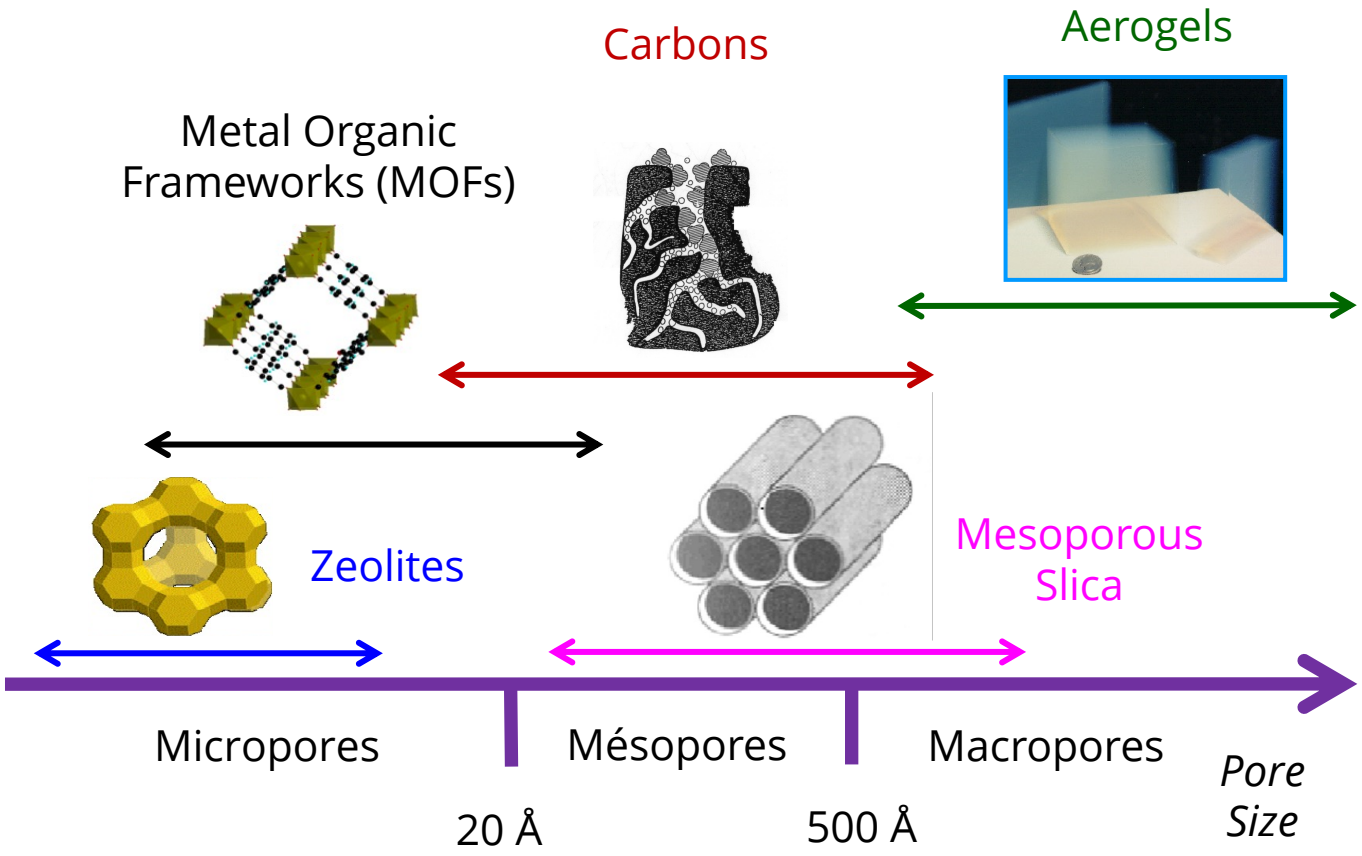


Absorption (Chimisorption): formation of carbamates

Fast & low-cost reaction

High energy consumption for regeneration
Limited stability (Solvent degradation) & Corrosion
Environmental & Health concerns

Porous solid materials



Large Diversity

- inorganic, organic and hybrid
- natural or man-made
- pores from 0.3 to 500 nm

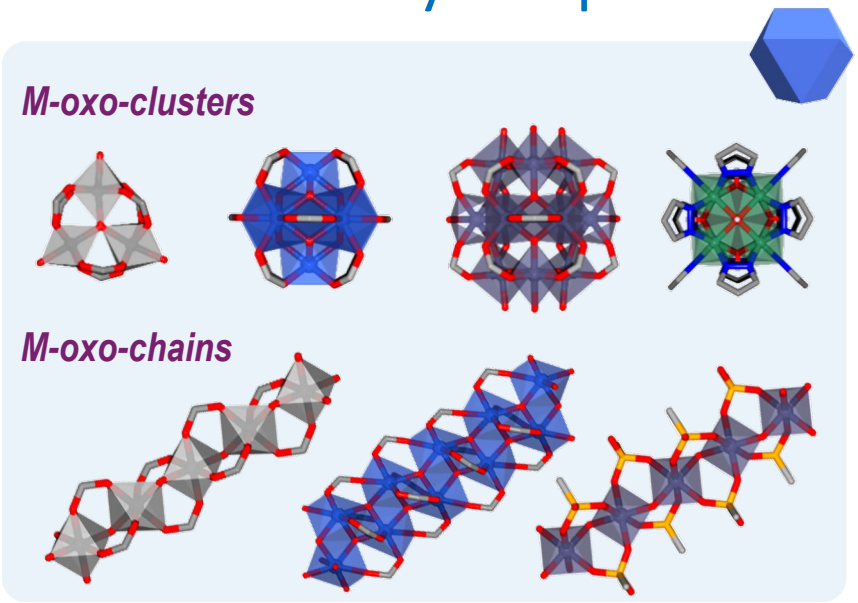
Societal Challenges

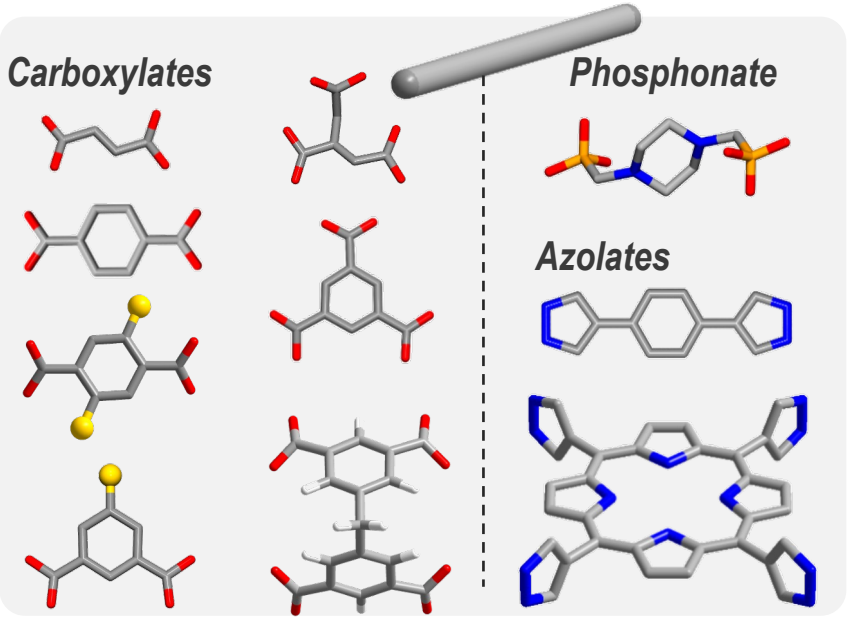
- (Indoor) air contaminant removal
- Drug Encapsulation/Release
- Humidity control-Heating-Air conditioning
- **CO_2 capture**

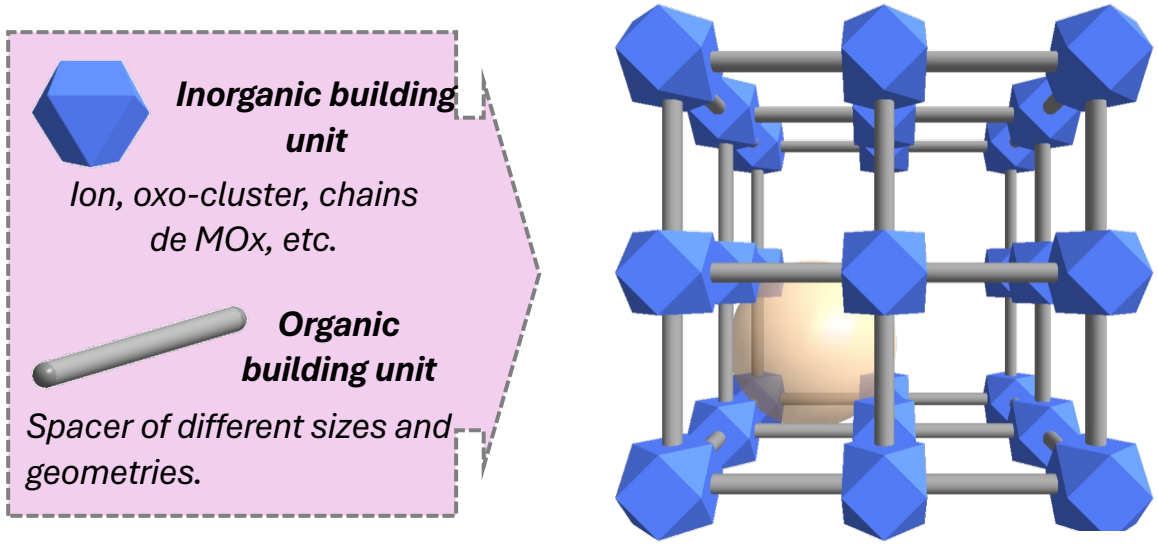
Needs of fine-tuned porous materials

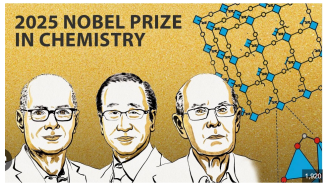
- Specific pore size, shape & chemical functionality
- Efficiency and durability under working conditions
- Exploitable at the industrial levels (shaping, scale-up…)

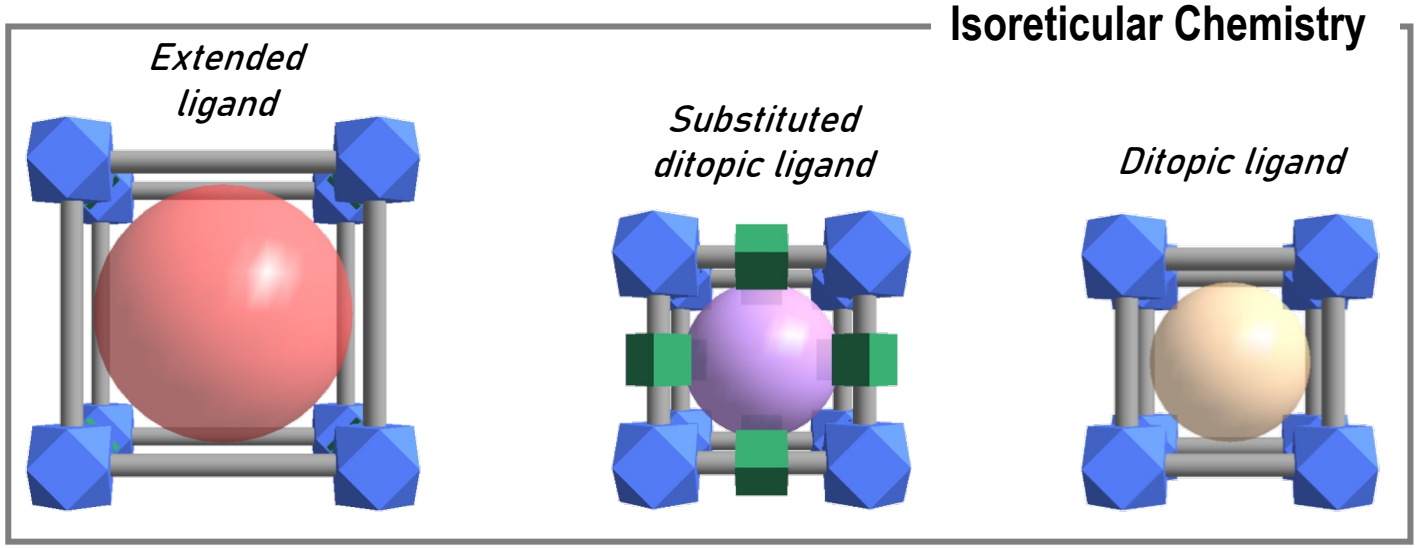
Hybrid porous materials: Metal Organic Frameworks (MOFs)







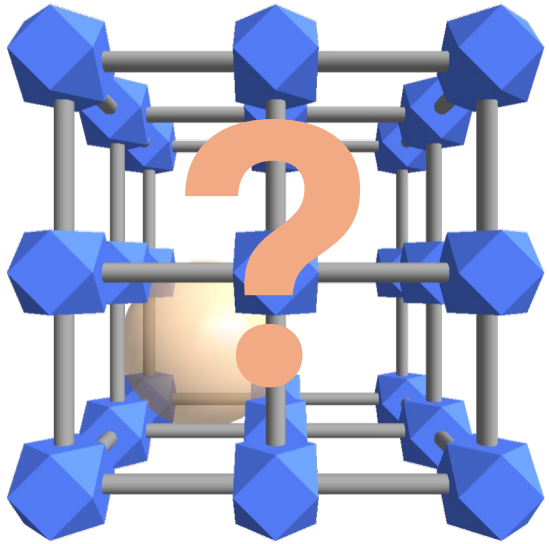


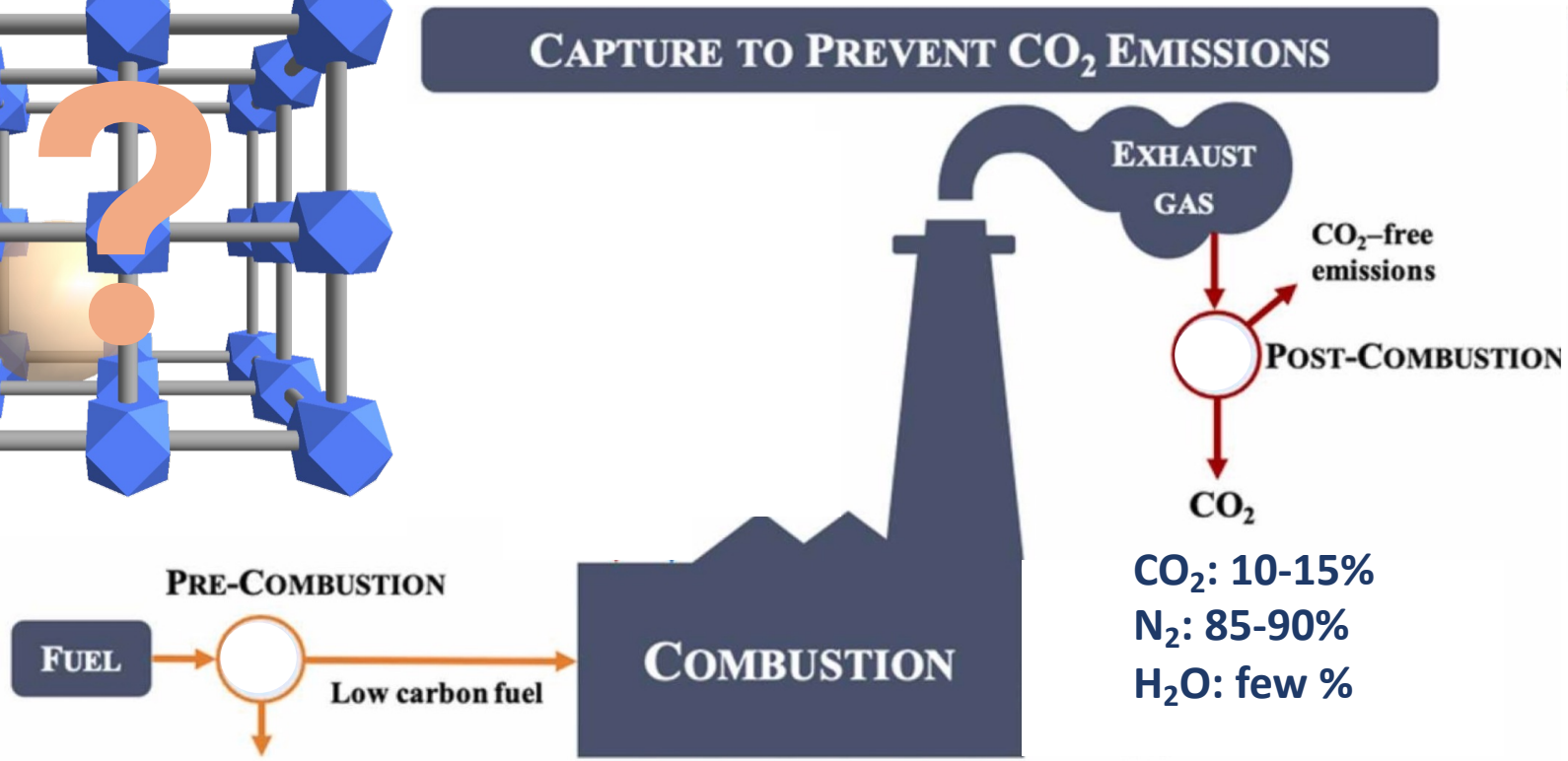


Multifunctional materials for Adsorption/Separation, Catalysis, ...

Van Speybroeck, Maurin, *MOF for a changing planet,* **Nature Materials** 2023

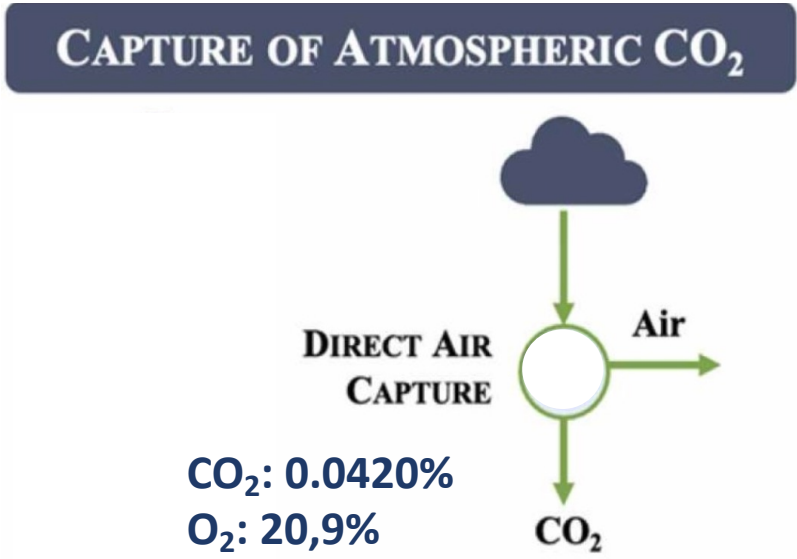
Design of optimal MOFs for CO_2 capture in distinct scenarios





Biogas/Natural gas
CO_2: 40-50%
CH_4 : 50-60%

CO_2: 10-15%
N_2: 85-90%
H_2O: few %



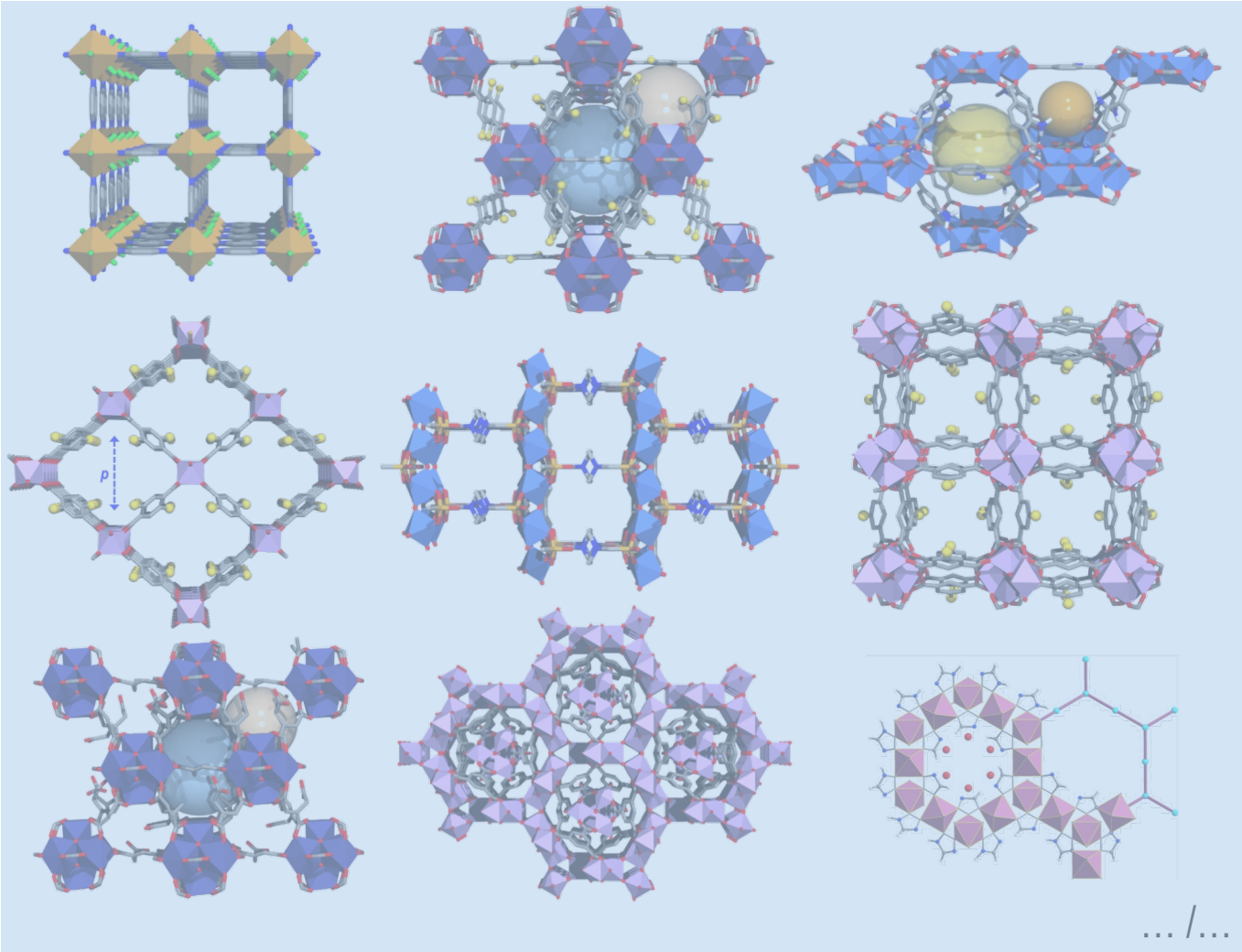
CO_2: 0.0420%
O_2: 20,9%
N_2: 78,1%
H_2O: various RH

(i) MOFs for post-combustion CO_2 capture (CO_2/N_2)

Systematic MOF computational screening (quantum chemistry & force field Monte Carlo)

MOF4AIR
IMAP INSTITUT DES MATÉRIAUX POREUX DE PARIS

Oxo-clusters
Chains
Sustainable metals: Ni^{2+}, Zn^{2+}, Al^{3+}, Zr^{4+}, Ti^{4+}….
Cost-effective linkers: carboxylates, furane….
Polar/Apolar functional groups
Hydrophobic/Hydrophilic
Cages
Channels
ultra-micro pores (0.3 to 0.6 nm)
micro-pores (< 2.0 nm)
Rigid/Flexible



Prediction-Understanding-Rationalization

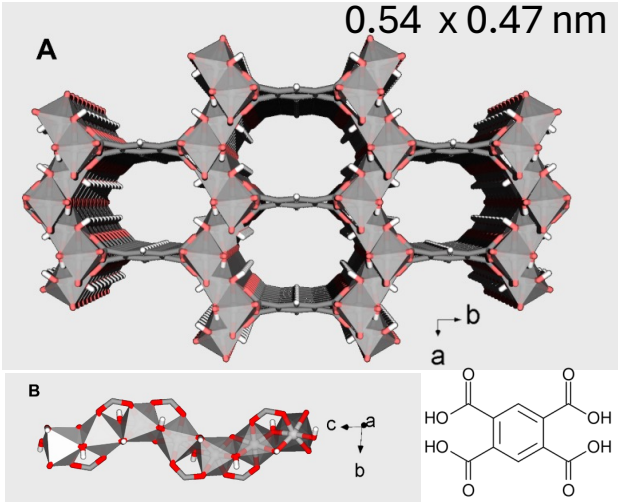
CO_2 adsorption isotherm,
CO_2/N_2 selectivity (binary mixture)
CO_2 affinity ($Q_{st,0}$)-preferential sittings
Structure-Property relationships

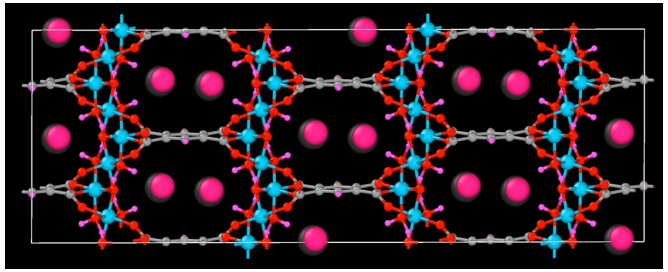
Promising MOF adsorbents for CO_2/N_2 separation

(i) MOFs for post-combustion CO_2 capture (CO_2/N_2)

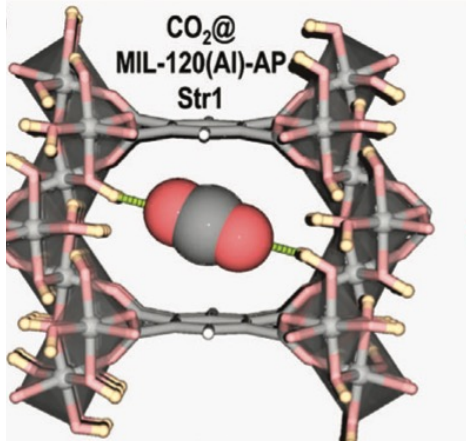
Ultra-microporous MIL-120(Al)

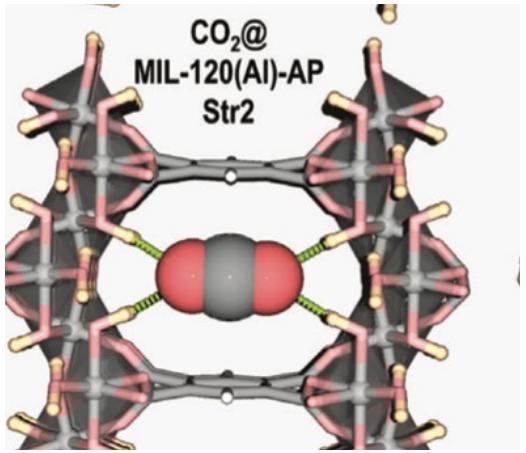
Confinement-driven capture



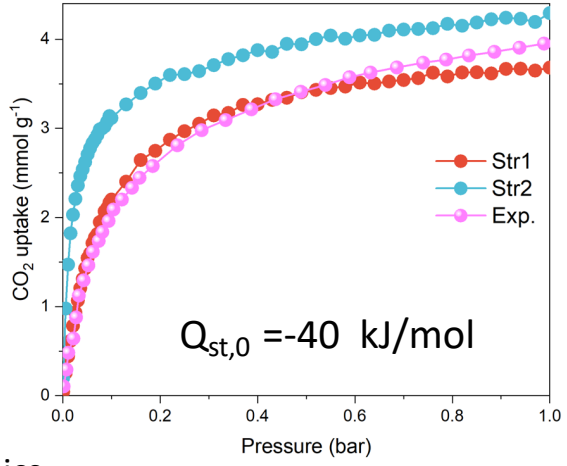


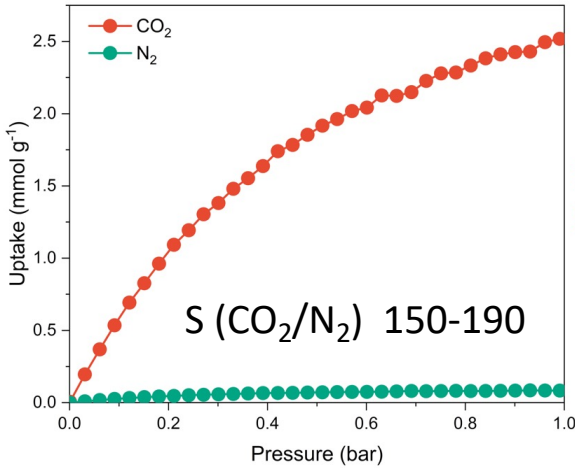
Machine Learning Potential Molecular Dynamics



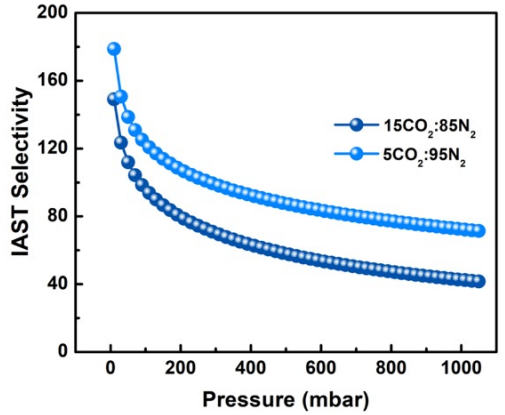


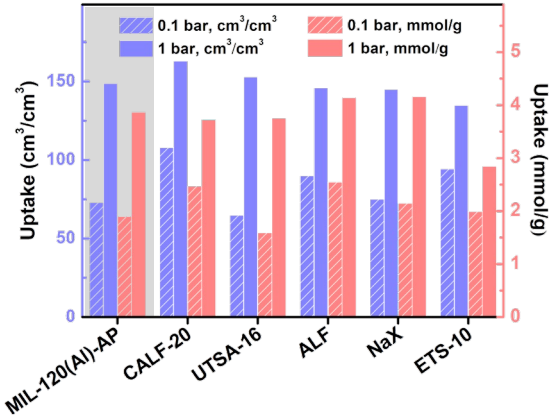
Density Functional Theory calculations





Monte Carlo simulations



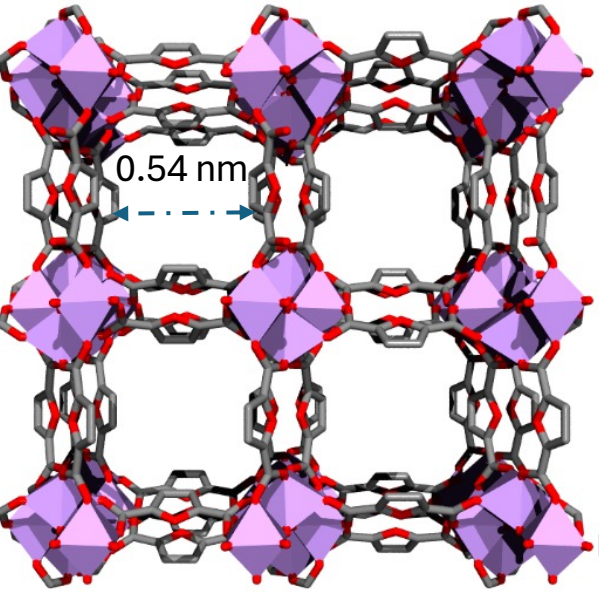


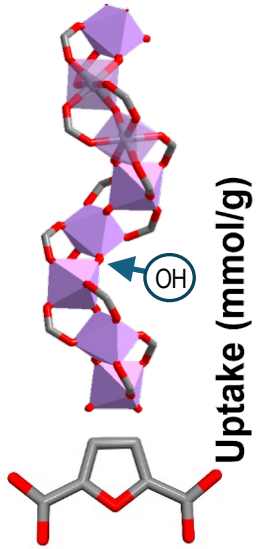
Hydrothermal synthesis
10 €/kg

Maurin, Serre *et al.*, **Advanced Sciences** 2024
Maurin *et al*, **Nature Commun** 2025

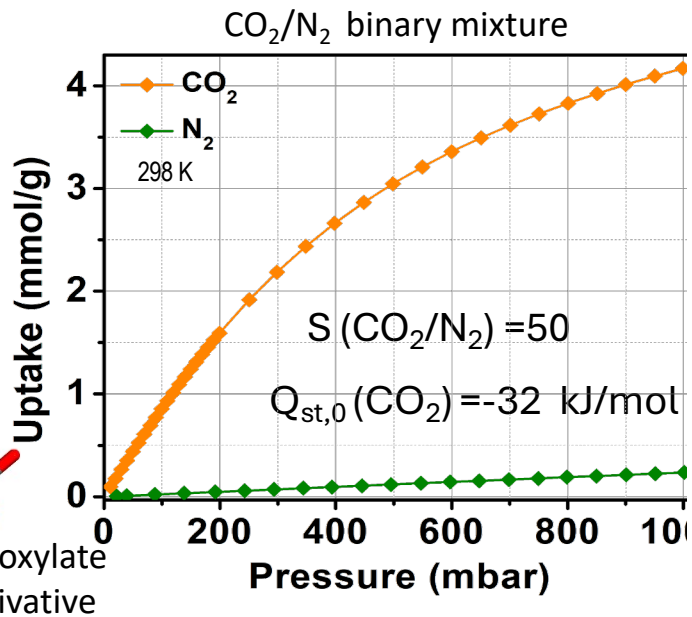
(i) MOFs for post-combustion CO_2 capture (CO_2/N_2)

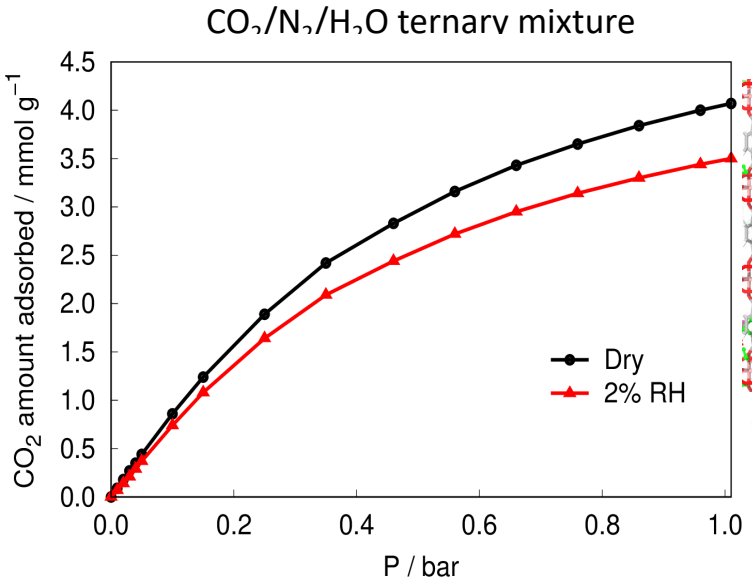
Ultra-microporous MIL-160(Al)

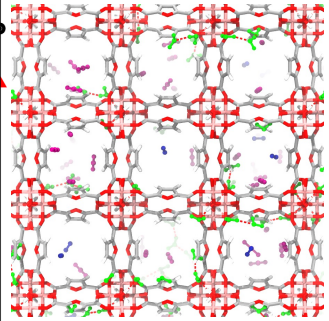




Furane dicarboxylate
Bio-mass derivative







CO_2 N_2 H_2O

Hydrothermal synthesis
15-20 €/kg

Shaping in beads

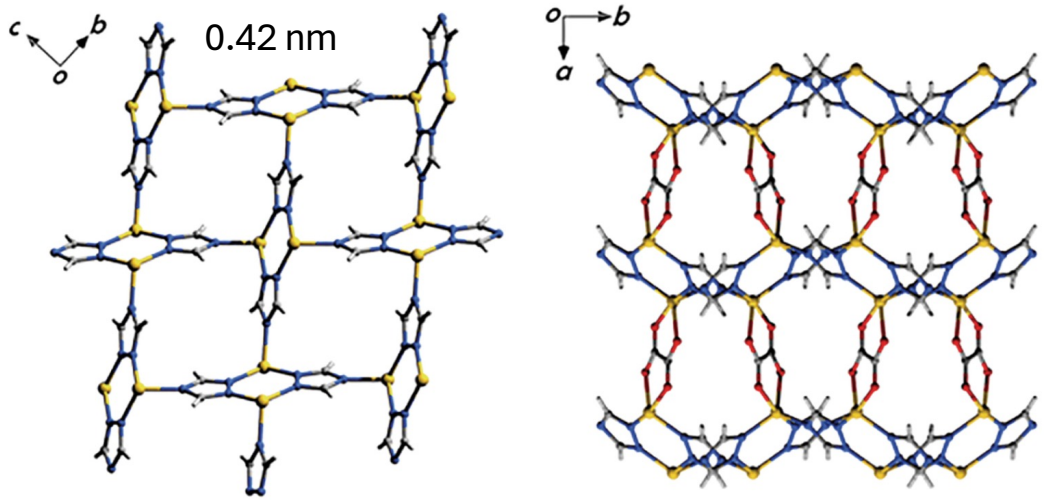
Industrial pilot VPSA, TCM (Norway)

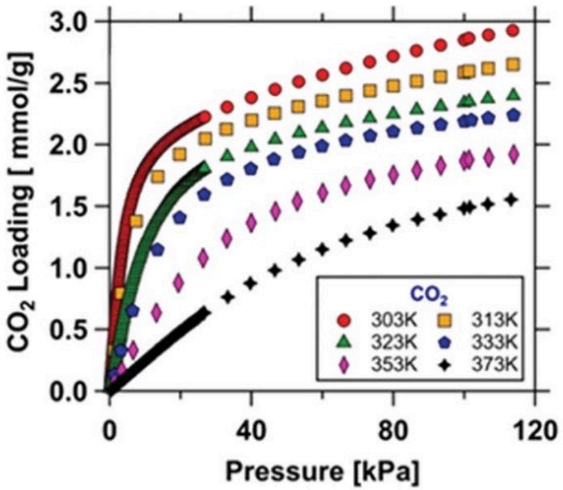
- 60 kg MIL-160(Al)
- High S(CO_2/N_2) even with few % H_2O
- Purity >95 %

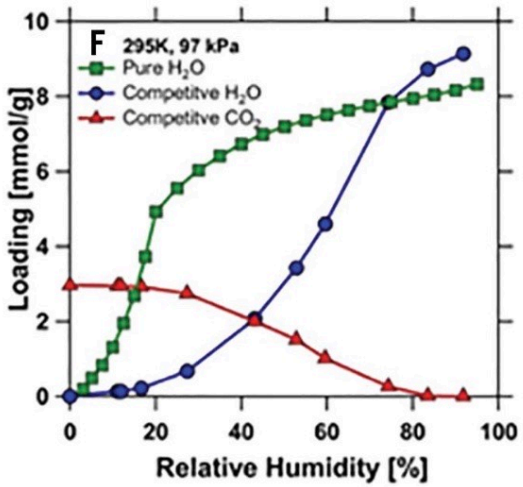
TECHNOLOGY CENTRE MONGSTAD

(i) MOFs for post-combustion CO_2 capture (CO_2/N_2)

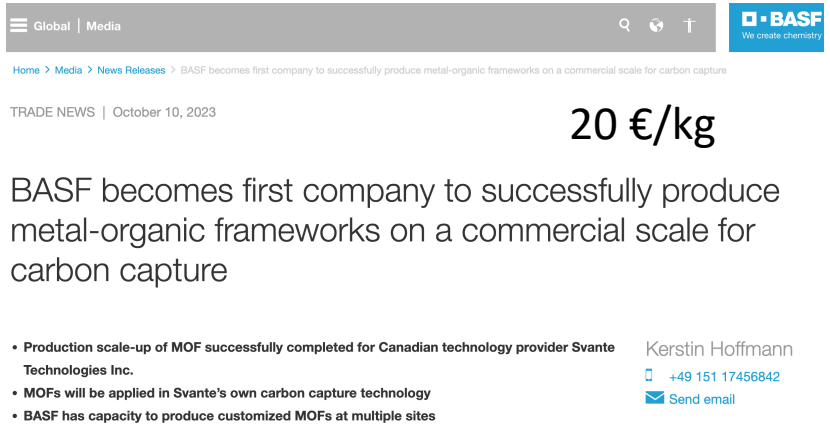
Ultra-microporous CALF-20(Zn), first MOF to reach industrial deployment for CO_2 capture







Zn_2(1,2,4-triazolate)$_2$(oxalate) MOF: robust, low-cost green synthesis, effective CO_2 capture in presence of humidity (RH=25%)


Global | Media

BASF We create chemistry

Home > Media > News Releases > BASF becomes first company to successfully produce metal-organic frameworks on a commercial scale for carbon capture

TRADE NEWS | October 10, 2023

20 €/kg

BASF becomes first company to successfully produce metal-organic frameworks on a commercial scale for carbon capture

- Production scale-up of MOF successfully completed for Canadian technology provider Svante Technologies Inc.
- MOFs will be applied in Svante's own carbon capture technology
- BASF has capacity to produce customized MOFs at multiple sites

Kerstin Hoffmann
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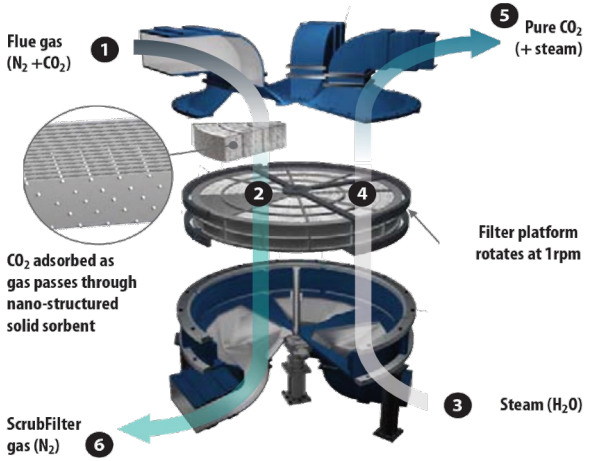


Cement plants, Portland, CO
→ 30 ton CO_2/day,
→ 45 € /ton CO_2

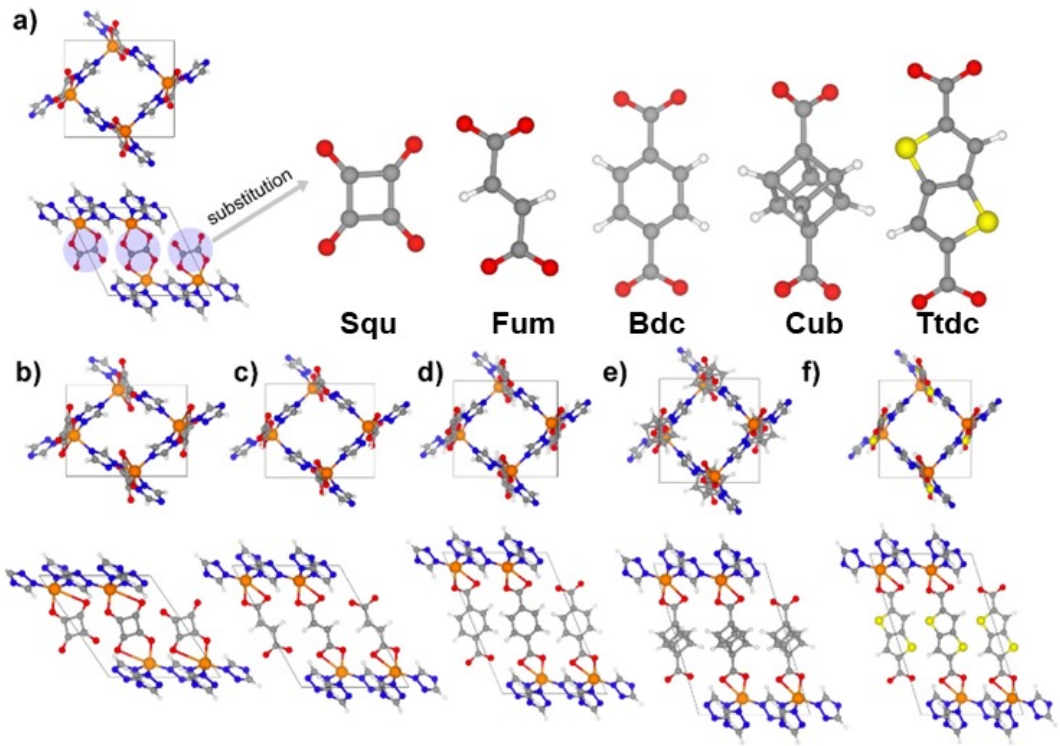
Ton-scale production & Svante commercial large-scale CO_2 capture rotating modules for cement plants, refineries…

Shimizu *et al.*, **Science** 2021

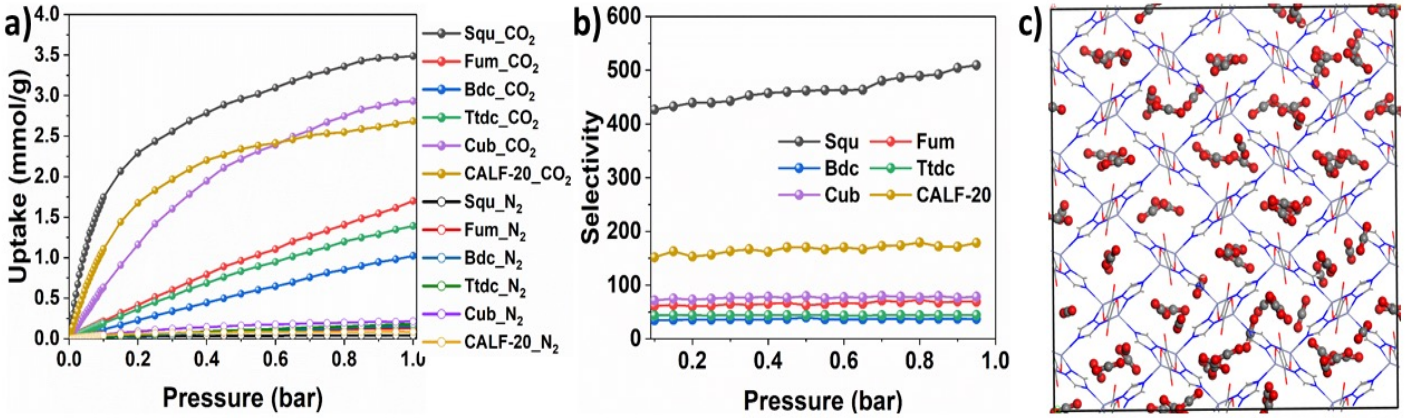
(i) MOFs for post-combustion CO_2 capture (CO_2/N_2)

Boosting CO_2 capture performance of CALF-20

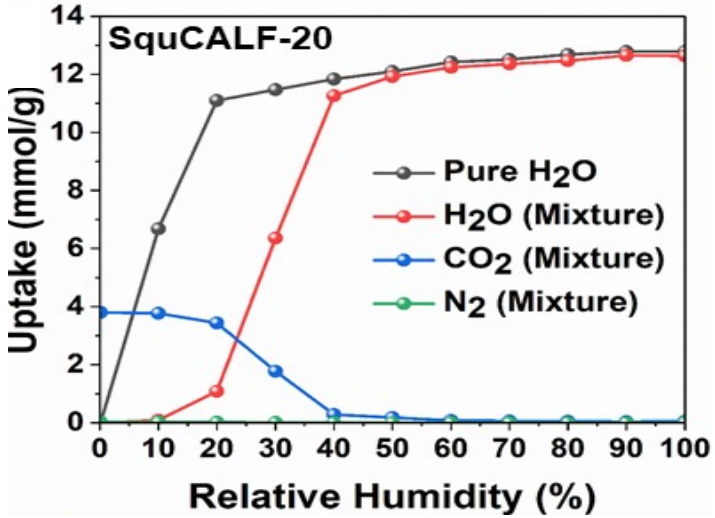
In silico generation of an isoreticular series



CO_2/N_2 separation in dry conditions



CO_2/N_2 separation under humidity



Most promising MOF: Squ-CALF-20

→ High CO_2 affinity: $Q_{st,0}$ (CO_2) =-38 kJ/mol

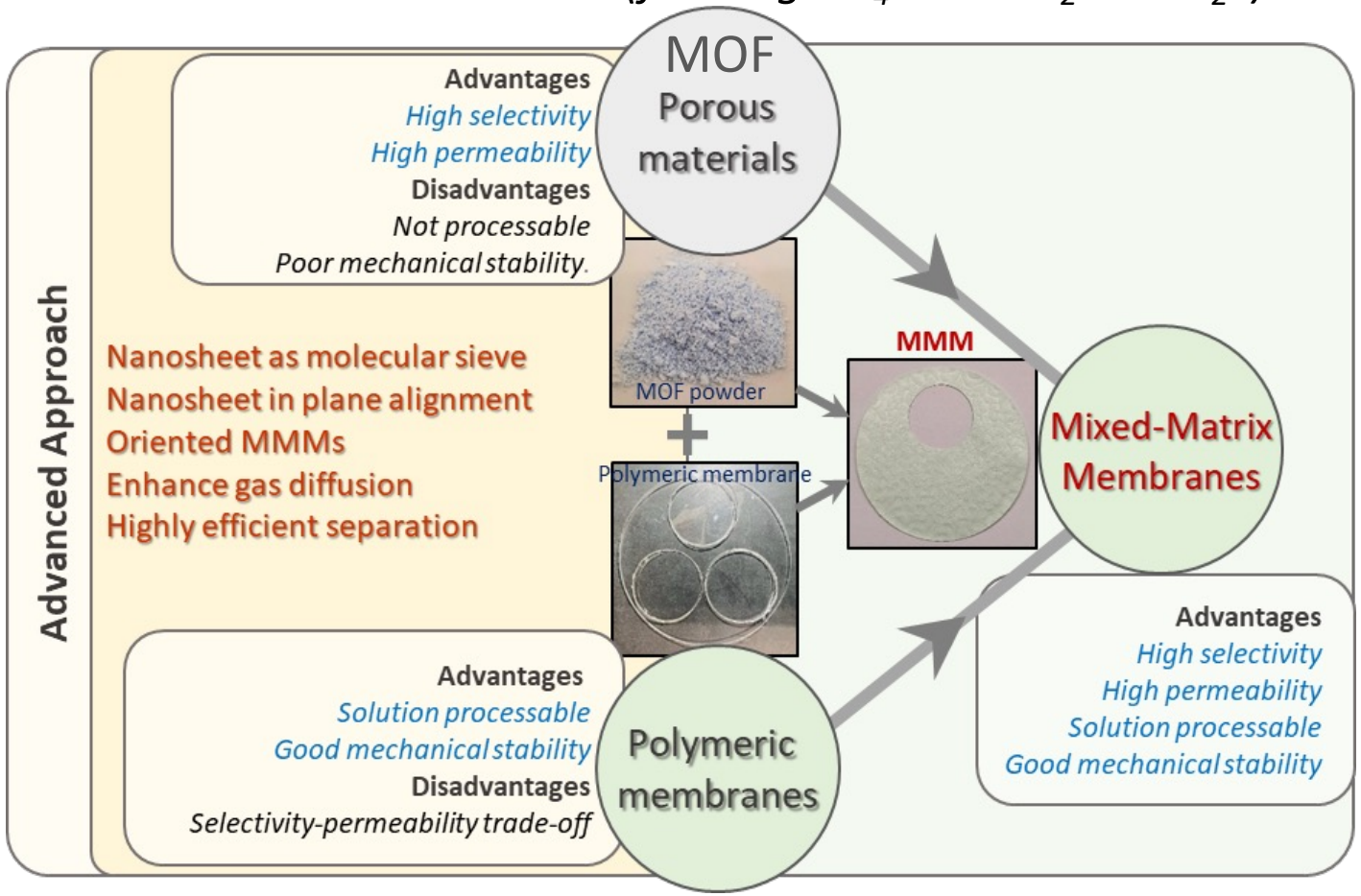
→ High S(CO_2/N_2) & Large CO_2 uptake maintained up to RH 20%

Maurin *et al*, **ACS App. Eng. Mater.** 2024, Maurin *et al* **Nature Commun** 2024

(ii) MOFs for pre-combustion CO_2 capture (CO_2/CH_4)

Mixed Matrix Membranes (MMMs) for **natural gas processing/Biogas upgrading**

MOF as a molecular sieves (filtering CH_4 over CO_2 and H_2S)

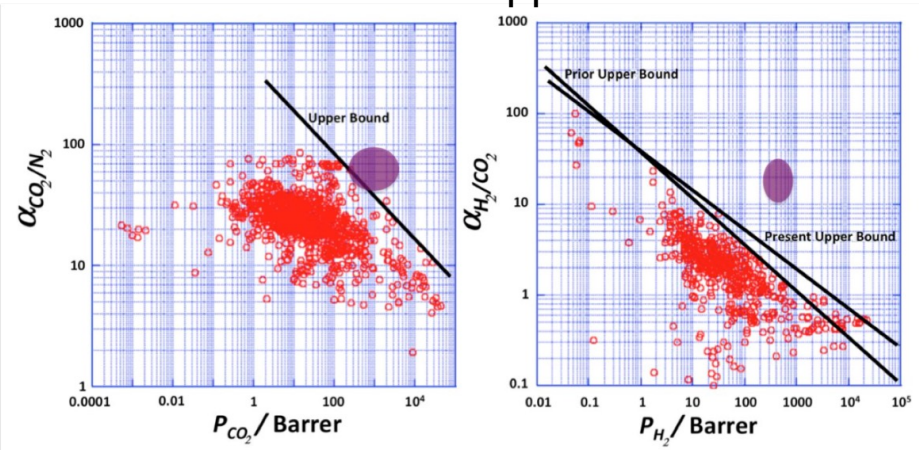


Eddaoudi *et al*, **Chem. Soc. Rev.** 2022; Maurin *et al*, **Chem. Sci.** 2025

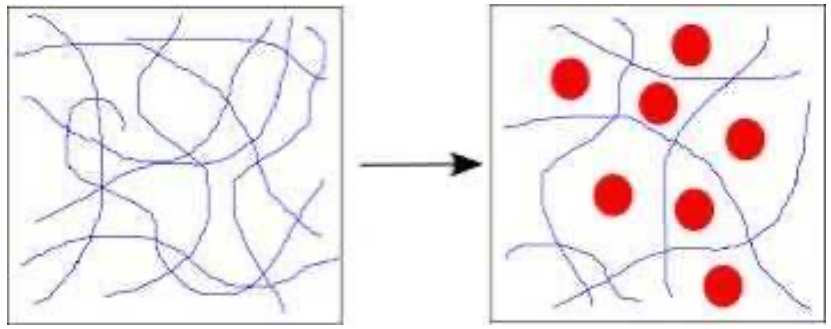
Overcome Pitfalls of pure polymer membranes

→ Trade-off between Permeability/Selectivity

Robeson's upper bound

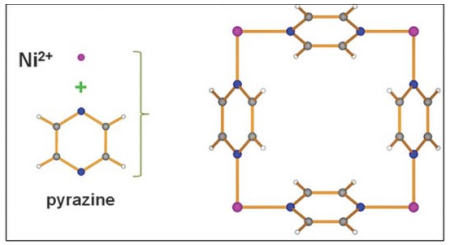


→ Plasticization



(ii) MOFs for pre-combustion CO_2 capture (CO_2/CH_4)

Ultra-small pore ALFFIVE-1-Ni (KAUST-8) as an *optimal molecular sieves* for CH_4 over CO_2 and H_2S



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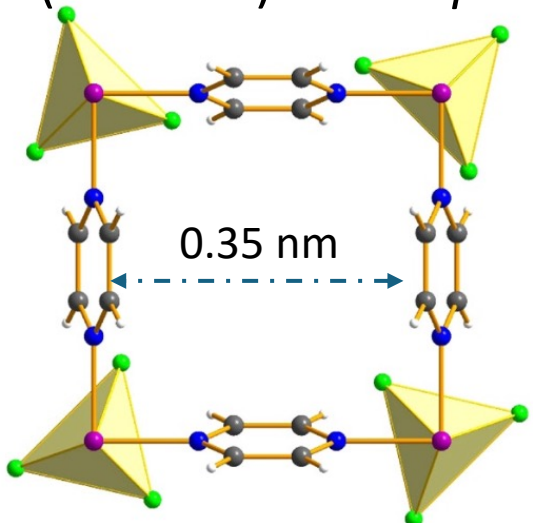
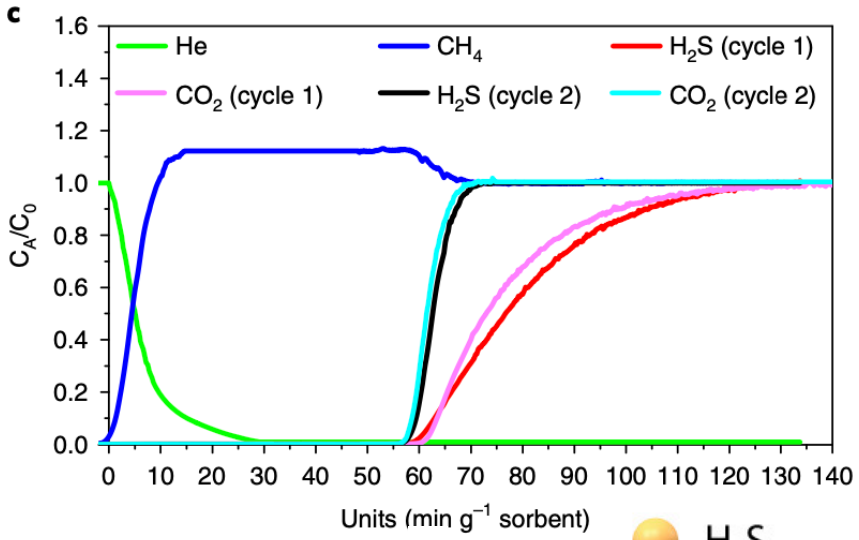
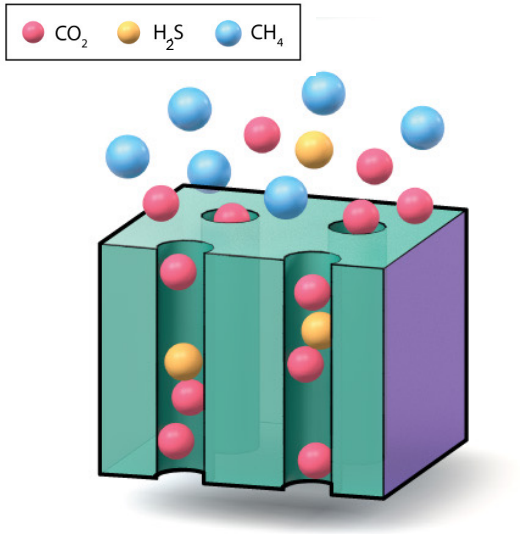
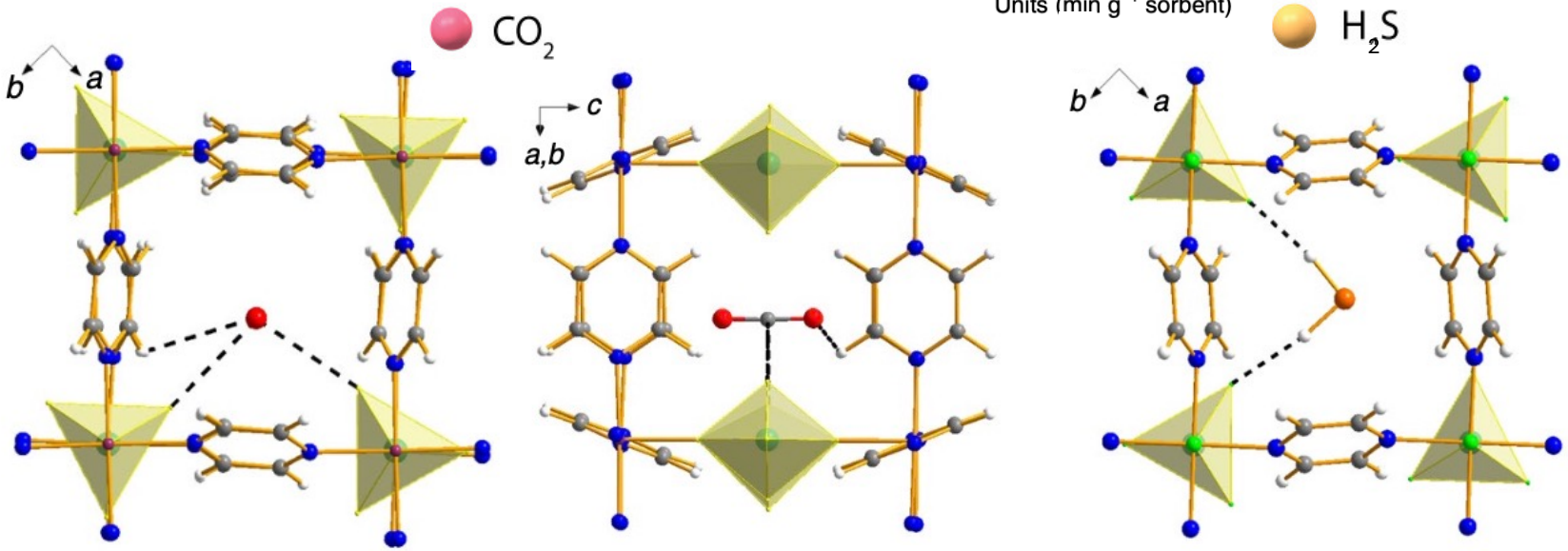








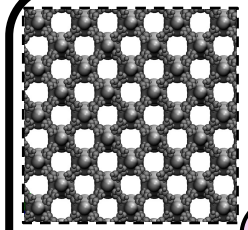
Maurin, Eddaoudi et *al* **Science** 2017

Maurin, Eddaoudi *et al* **Nature Energy** 2018

Density Functional Theory calculations

MOF Mixed Matrix Membranes: Our computational toolkit

MOF Surface model



Slab creation

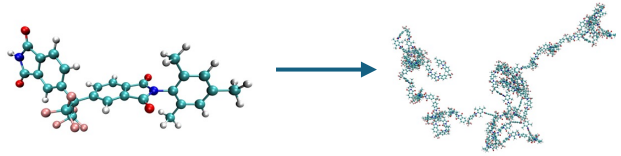
optimization

charge calculation

DFT

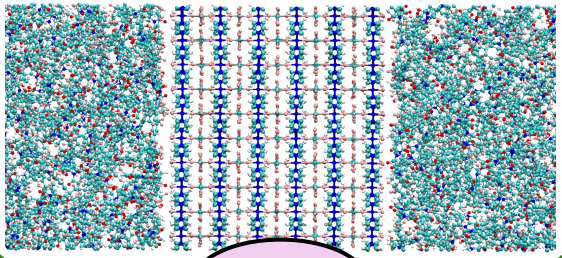
Polymer

Polymer atomistic model builder

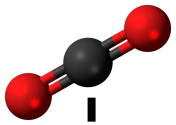


FF- EMD

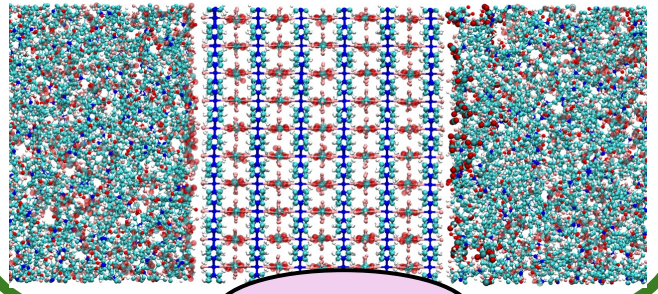
MMMs generation



FF-EMD

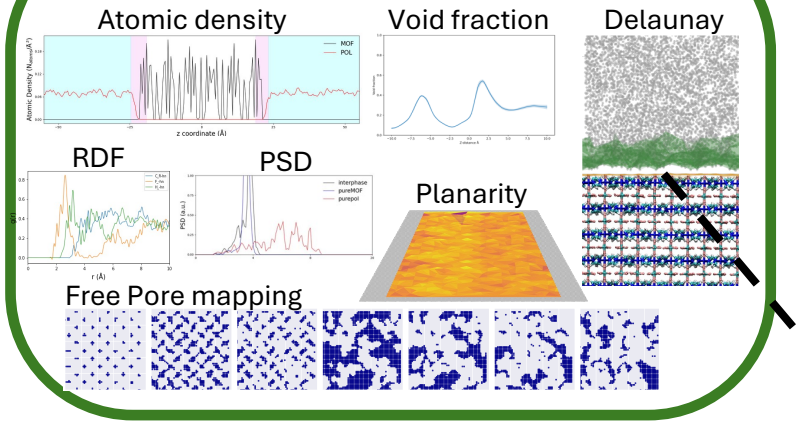


Gas Adsorption

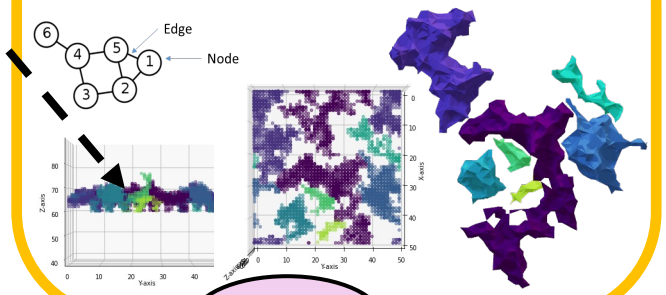


FF GCMC

Post analysis toolkit



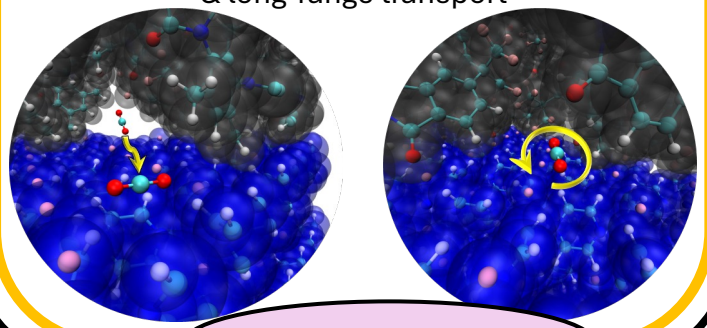
Graph Theory



NetworkX

Gas Dynamics

Interfacial (translation + rotation) reorientation & long-range transport

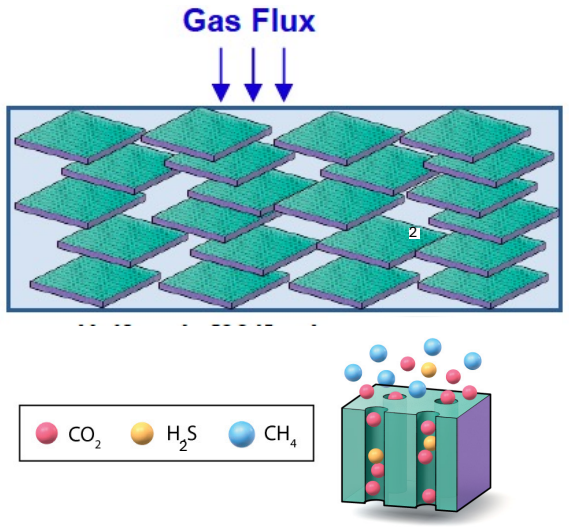


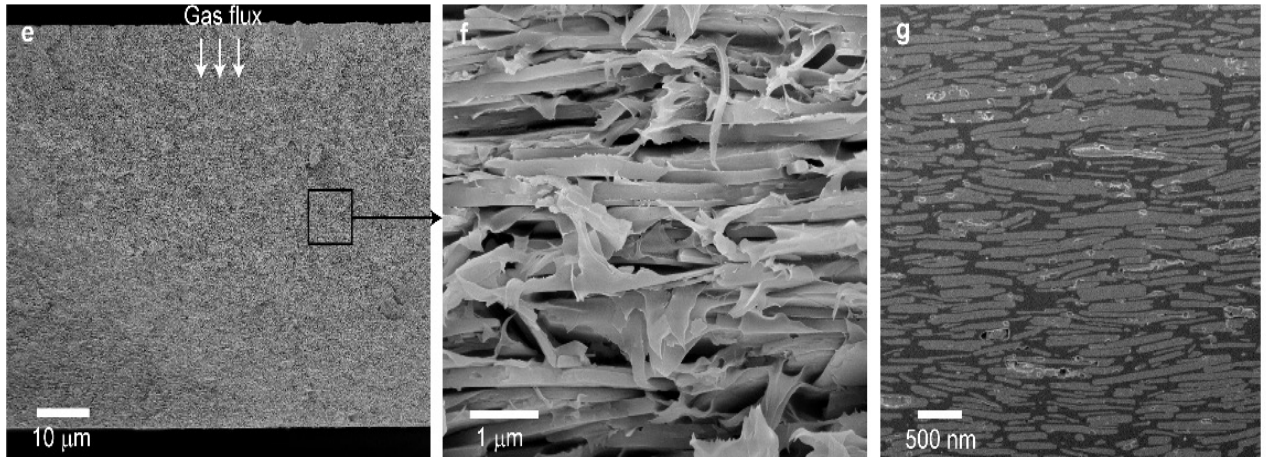
FF EMD & NEMD

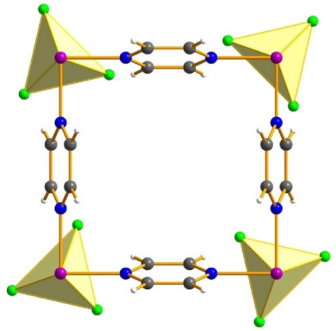
Maurin *et al*, **Chem. Sci.** 2025

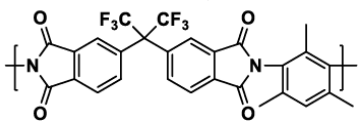
(ii) MOFs for pre-combustion CO_2 capture (CO_2/CH_4)

ALFFIVE-1-Ni/Polymer MMMs

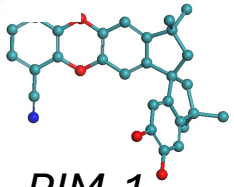




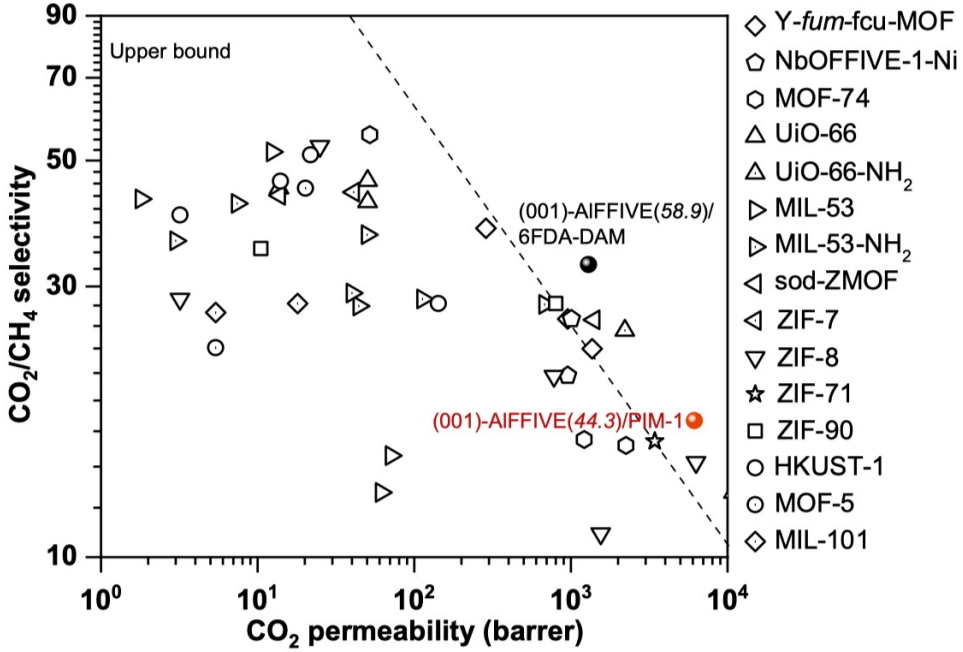




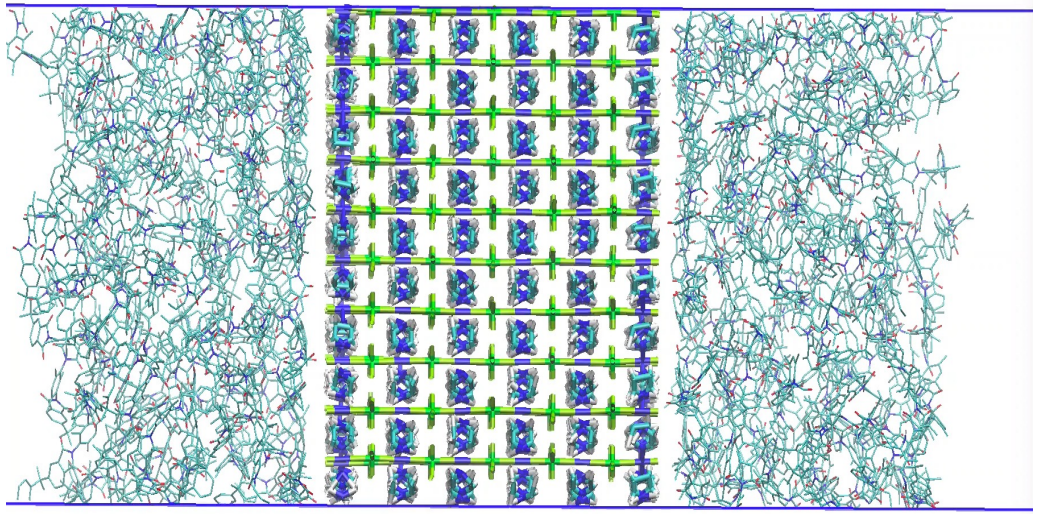
6 FDA-DAM



PIM-1

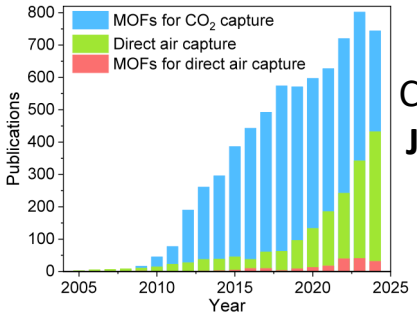


Molecular Dynamics simulations



Maurin, Eddaoudi *et al*, **Science** 2022
Eddaoudi, Maurin et al, **Science Advances** 2024

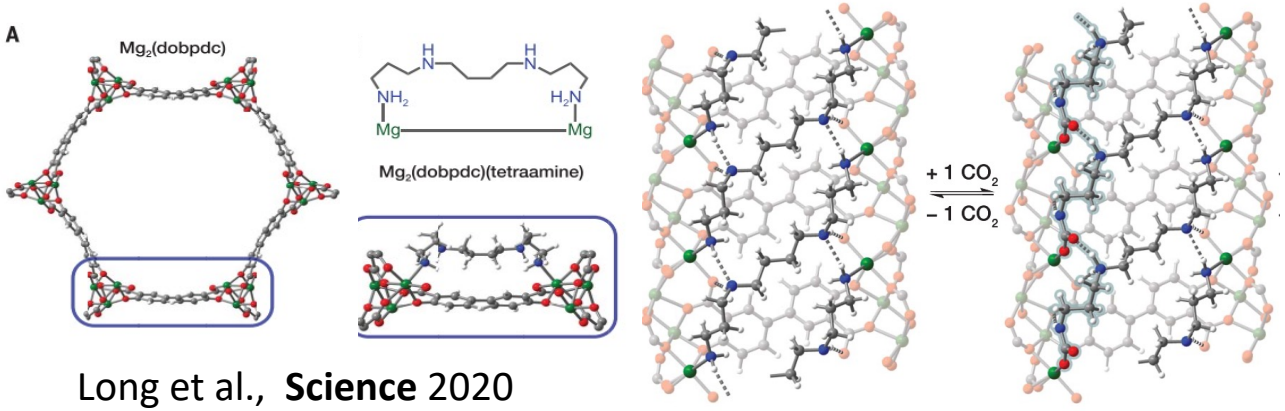
(iii) MOFs for direct air CO_2 capture



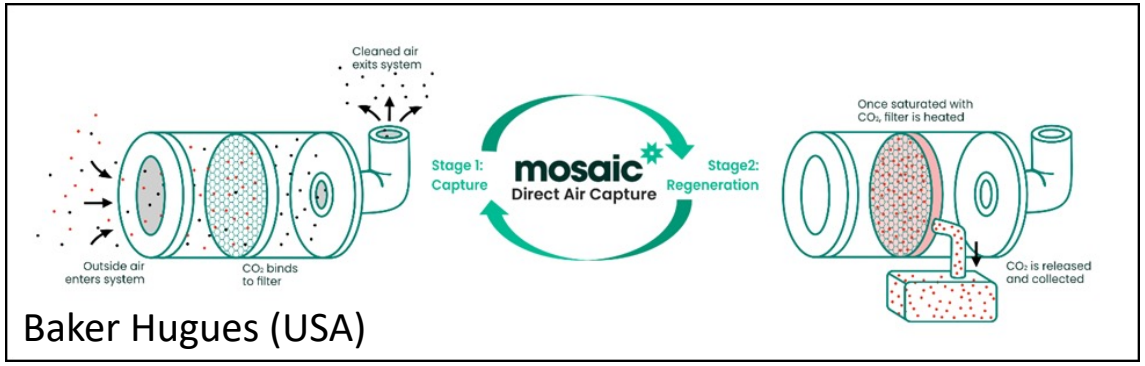
Chen et al, **JACS**2025

Strategy 1

Grafting Amine-functions to Open Metal Sites in Mesoporous MOFs for Chimisorption



Long et al., **Science** 2020



Baker Hugues (USA)

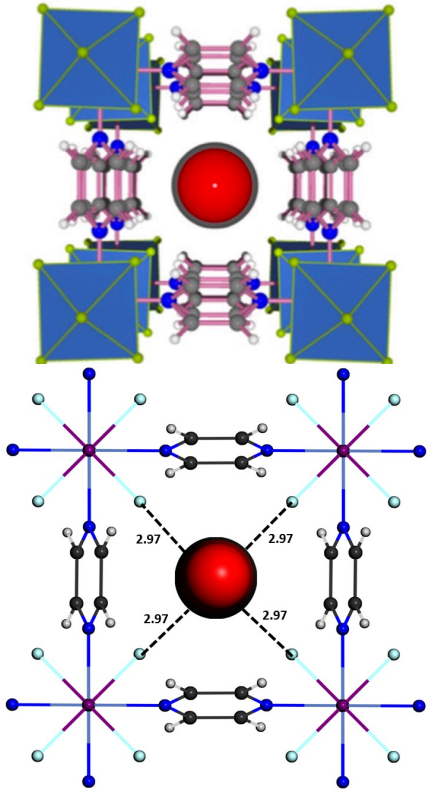
Effective, but what about stability and environmental impact?

Strategy 2

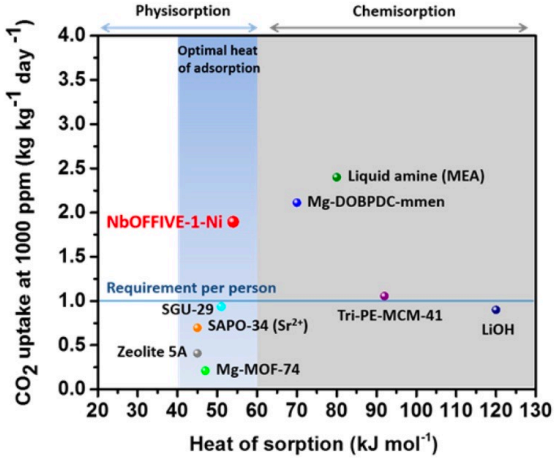
Ultra-small pore MOF for Physisorption

NbOFFIVE-1-Ni (KAUST-7) best MOF so far

Ni-pyrazine sql layers pillared by $NbOF_5$



Sweet-spot for CO_2 packing
→Pore size: 0.33 nm
→ F-arrays



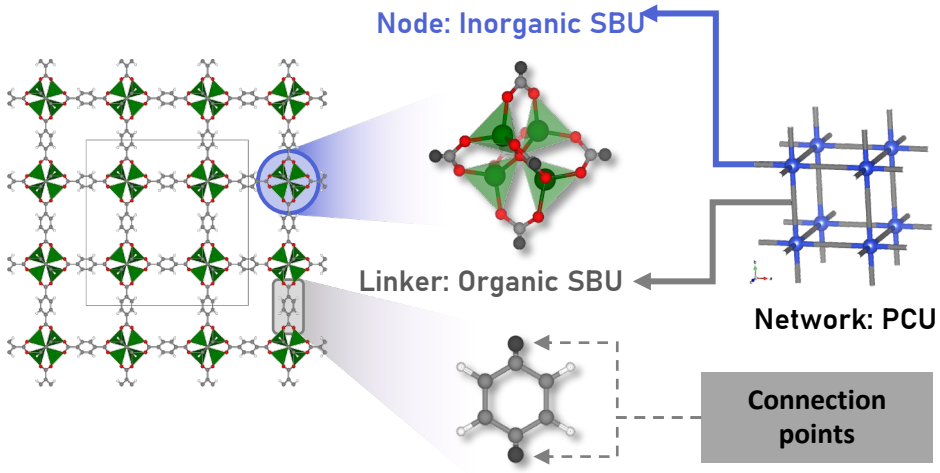
Effective, but competition with humidity is an issue

Eddaoudi, *al* ***JACS*** 2017
Maurin, Eddaoudi *et al* **Nature Energy** 2018

MOFs for direct air CO_2 capture: Artificial Intelligence-driven design

(1) Creation of new MOFs structure (hMOFs)

Secondary Building Unit (SBU) Assembly Approach



Tools and SBUs/topology datasets:

Structure creation

- PORMAKE
- PoAuToGraFS
- Zeo++
- ToBaCCo
- reMatMod.jl
- stk

SBUs database

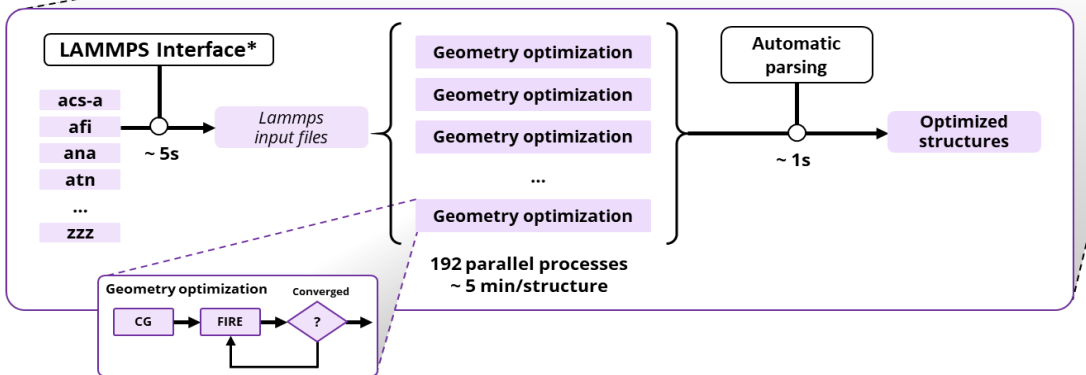
- Truly curated HEALED SBU: 952 inorganic and 568 organic cleaned SBUs

Topology database

- Reticular Chemistry Structure Resource (RCSR): *1D, 2D, and 3D networks*
- Merged-net Database >353 topologies with multiple linkers and nodes

Our Workflow

chemical/geometric features, SMILES, SELFIES...

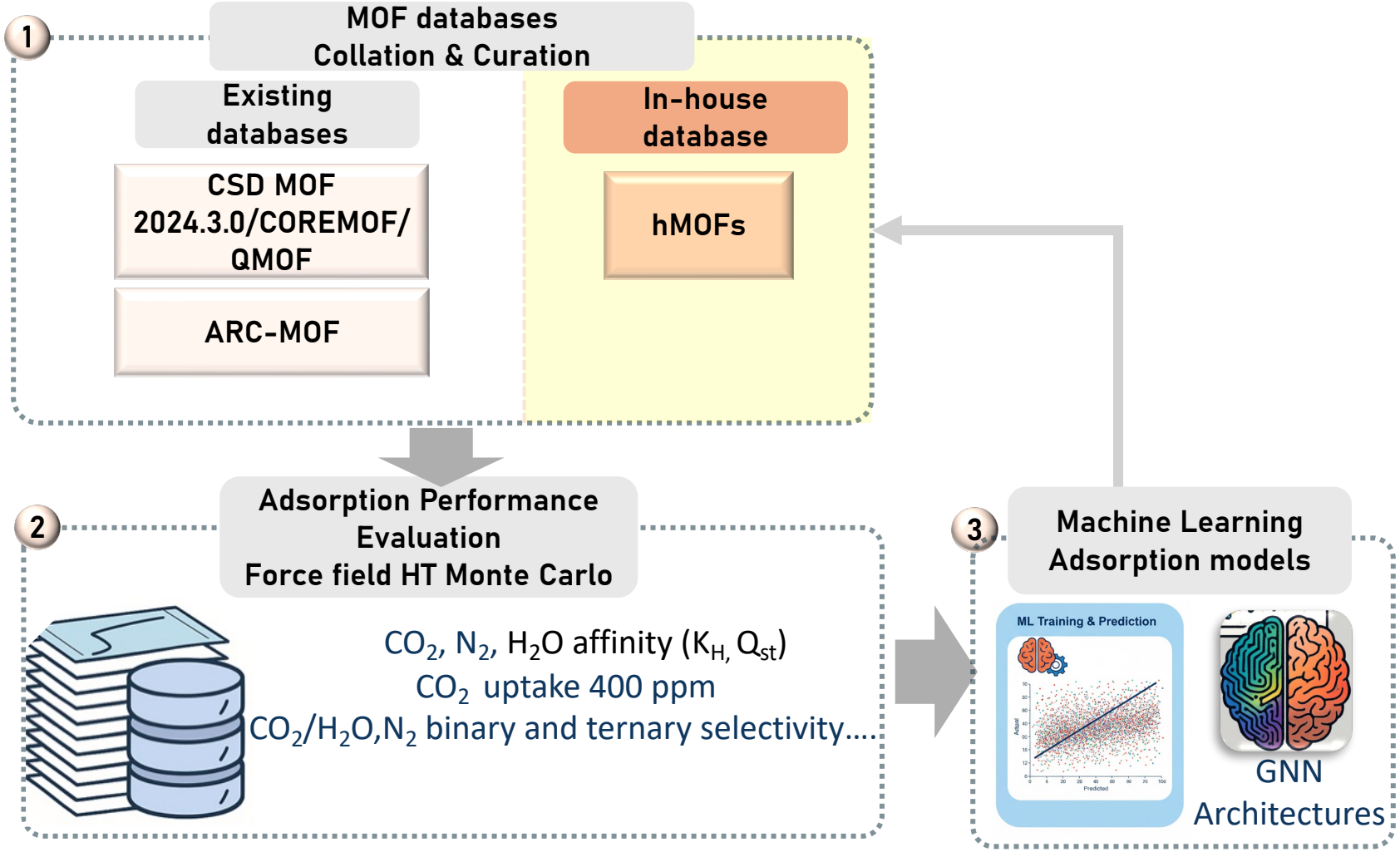


Millions of novel hMOFs
with less-explored topology/chemistry

Enhanced MOF structure landscape exploration

MOFs for direct air CO_2 capture: Artificial Intelligence-driven design

(2) Large scale CO_2 Adsorption Data: High-Throughput molecular simulations & Machine Learning models



MOFs for direct air CO_2 capture: Artificial Intelligence-driven design

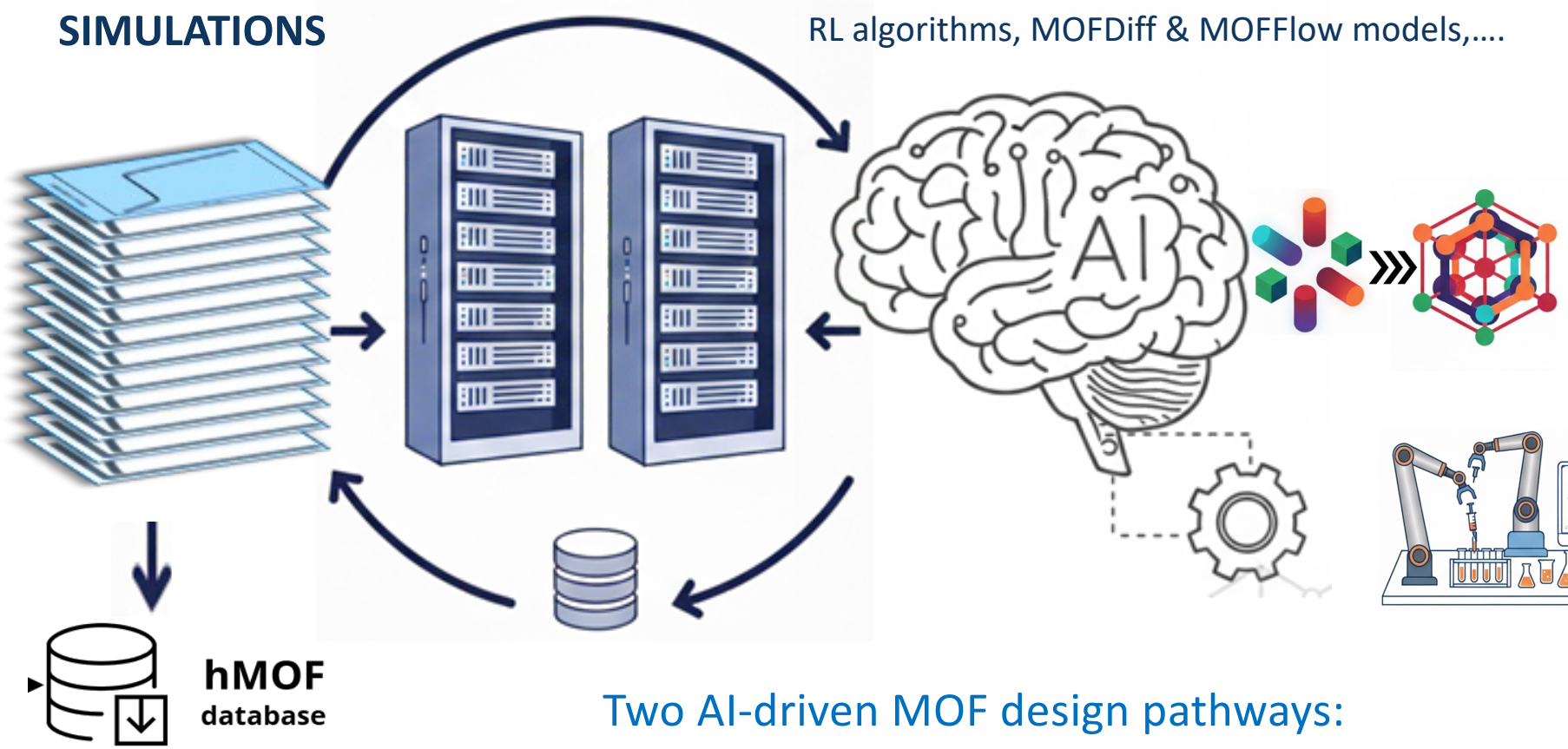
(3) From AI-design to MOF synthesis & adsorption testing

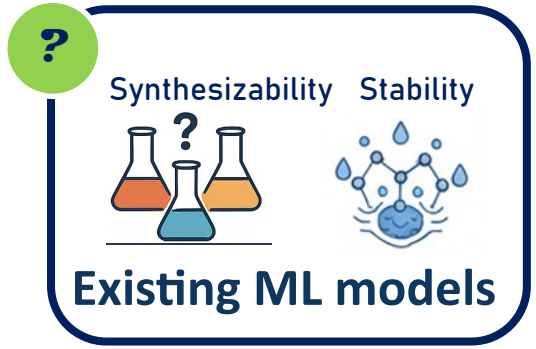
HT-MC-ML ADSORPTION SIMULATIONS

AI-INVERSE DESIGN

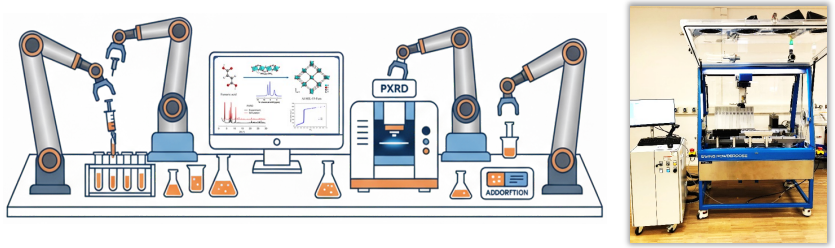
RL algorithms, MOFDiff & MOFFlow models,….

ML PREDICTION

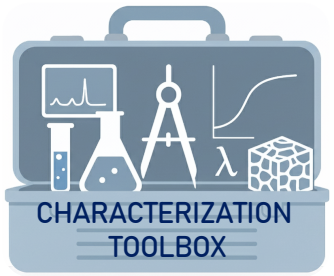




HT-ROBOTICS SYNTHESIS



PERFORMANCE EVALUATION



High performance hMOFs

Two AI-driven MOF design pathways:

→ Identification of high performance hMOF

→ AI-inverse design

Conclusions/Perspectives

CO_2 capture in post-combustion and pre-combustion conditions

Computational-aided identification of effective MOFs sorbents and MOFs-based membranes

Ongoing Industrial Applications of MOFs for CO_2 capture in post-combustion (cement plants)

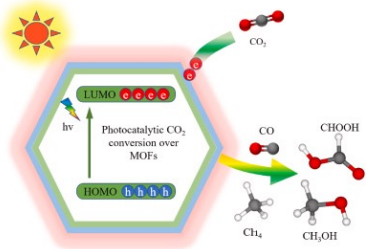
Direct Air CO_2 Capture

Effective amine-grafted MOFs for chimisorption, durability?

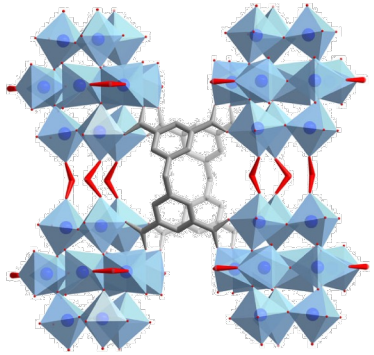
Deployment of AI-tools to design new ultra-small pore MOFs for physisorption

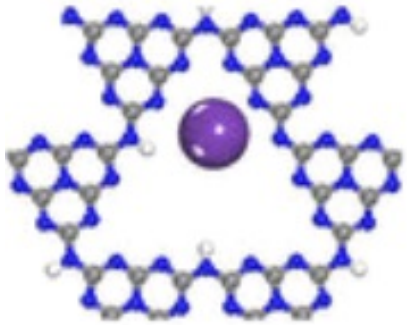
Beyond Capture……Conversion

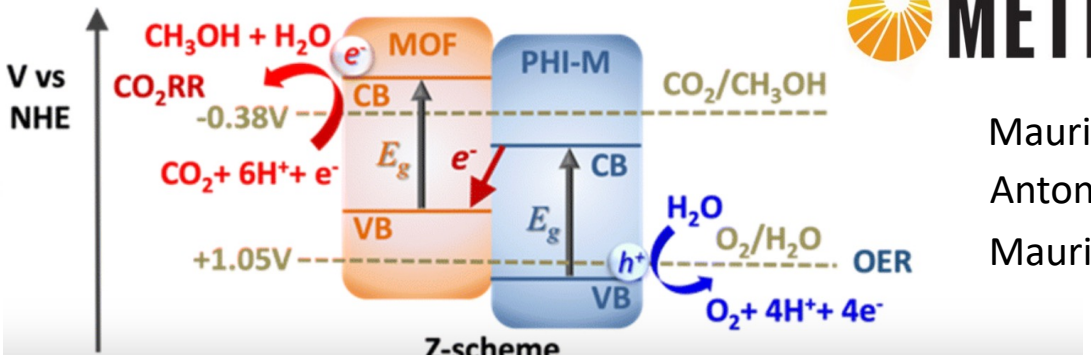
Ongoing development of MOF-based composites photocatalysts for CO_2 reduction



Metalated Cu@MIP-177(Ti) (CO2RR)/Metal doped g-C_3N_4 (OER)







METHASOL
CO_2 TO CH_3OH

Maurin, *et al* **Chem. Sci** 2024

Antonietti, Maurin et al, **ACS Catalysis** 2025

Maurin, Antonietti *et al* **ACS Catalysis** 2025

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D. Fan, S. Liu, F. Lopes Oliveira, M. Wahiduzzaman

Dr. C. Serre *et al*

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Prof. M.Eddaoudi *et al*,
Prof. B. Ghanem *et al.*
Prof. J. Schmidhuber *et al.*

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