MOST-H2

Novel metal organic framework adsorbents for efficient storage of hydrogen

Project Overview

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Grant Agreement No: 101058547

General information

- **MOST-H_2** stands for “Novel metal organic framework adsorbents for efficient storage of hydrogen”
- Research and Innovation Action
- Project budget: 4.9 M€
- Project duration: 48 months (June 2022 - May 2026)
- Consortium consists of 16 partners from 8 countries: Greece, Germany, Spain, the UK, Austria, France, Italy, Morocco
- Project coordination: National Center for Scientific Research “Demokritos”, Greece

https://most-h2.eu/

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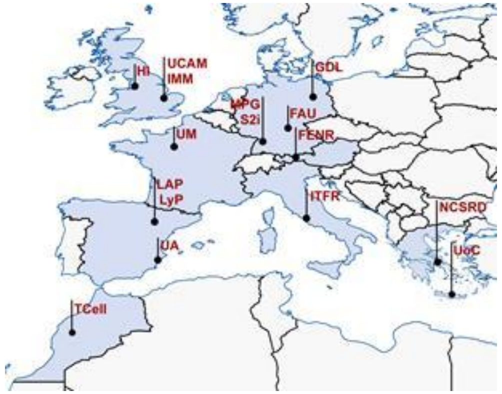
The MOST-H2 consortium



UNIVERSITIES

- University of Crete - Greece
- Le Mans Université - France
- Friedrich-Alexander-Universität Erlangen-Nürnberg - Germany
- Universidad de Alicante - Spain
- Université Mohammed VI Polytechnique – Morocco
- University of Cambridge - UK

Research Centers

- NCSR Demokritos - Greece
- Max Planck Institute for Intelligent Systems - Germany

Private sector

- Laguens y Perez S. L. - Spain
- Lapesa Grupo Empresarial S. L. - Spain
- FEN Research GmbH - Austria
- Italferr S.p.A. - Italy
- GreenDelta GmbH – Germany
- Steinbeis 2i GmbH – Germany
- Immaterial Ltd - UK
- Hiden Isochema Ltd - UK

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H_2 storage technologies

Physical storage

- Compressed gas
- Liquid H_2
- Cryo-compressed H_2

Very high pressures or/and very low temperatures

Material-based storage

Absorption

- Metal hydrides
- Chemical storage
  NH_3, NH_3BH_3, LOHCs etc

Elevated temperatures

Adsorption

- Large surface area materials (extended fluid-solid interface)
- Nano-confinement (different behavior compared to the bulk)
- Moderate pressure
- Cryogenic conditions

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Design computationally, synthesize and experimentally validate new nanoporous adsorbents for solid state hydrogen storage

- Development of new Metal Organic Frameworks with **usable H_2 storage capacities of at least 10 wt% and 50 g/L below 100 bar**

- Develop a **cryo-adsorption H_2 storage system** delivering up to **500 g of H_2** / testing in a relevant environment

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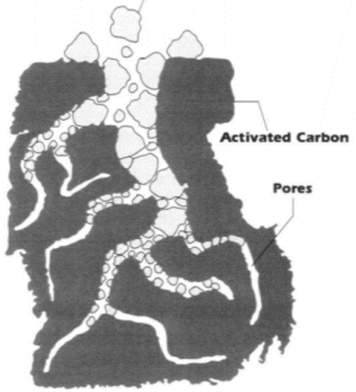
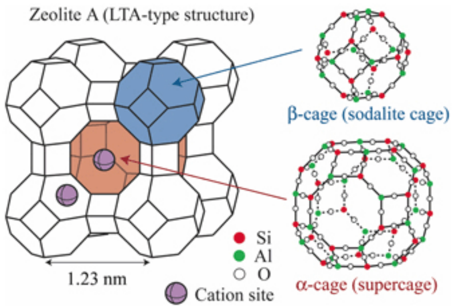
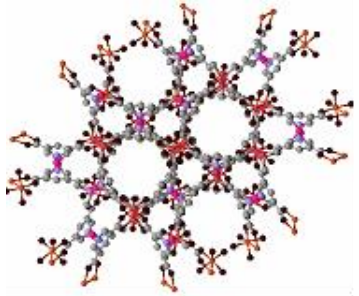
MOFs vs other nanoporous adsorbents





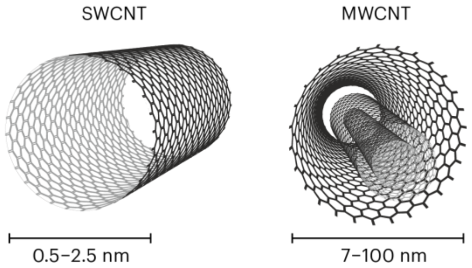


Porous carbons

- BET areas <4000 m^2/g → H_2 storage capacity < 7-8 wt% at material level (rarely > 6 wt%)
- Produced by pyrolysis of amorphous precursors (coals, agricultural by-products, etc.) → highly disordered pore structure and surface chemistry → difficult to accurately tailor pore size/shape to optimise H_2 adsorption
- Ordered structures are very costly due to complex synthesis

Silicas, zeolites, CNTs

- Cheap and robust but low BET areas (< 1000 m^2/g)
- Carbon nanostructures (nanotubes, graphene) or 2d materials have not shown adequate H_2 storage performance – poor reproducibility of results



Metal Organic Frameworks

- BET areas >5000 m^2/g
- H_2 adsorption capacities > 10 wt%
- Can be rationally designed following reticular chemistry rules (carefully selected building blocks can provide molecularly engineered pore networks)

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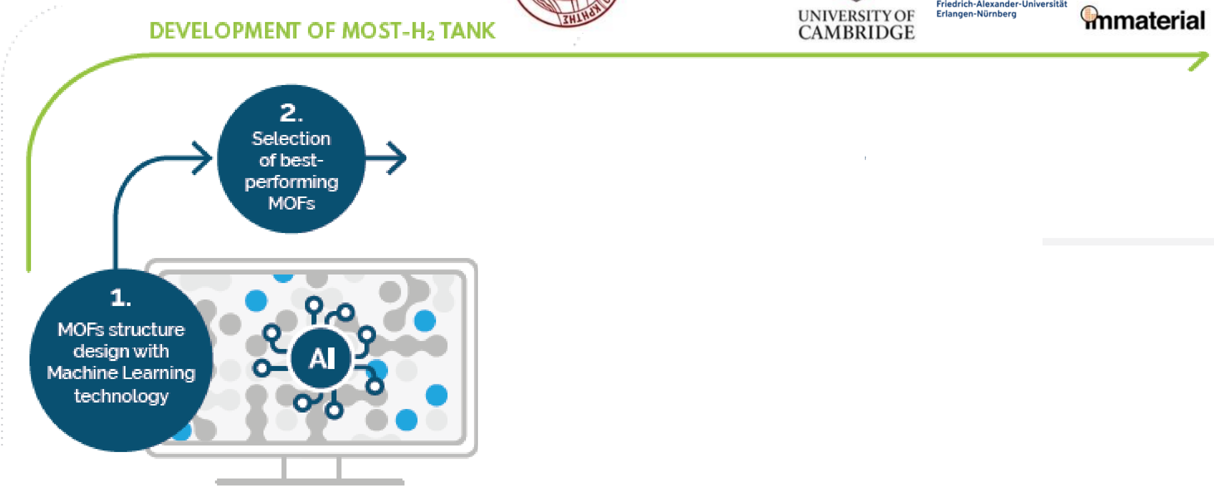
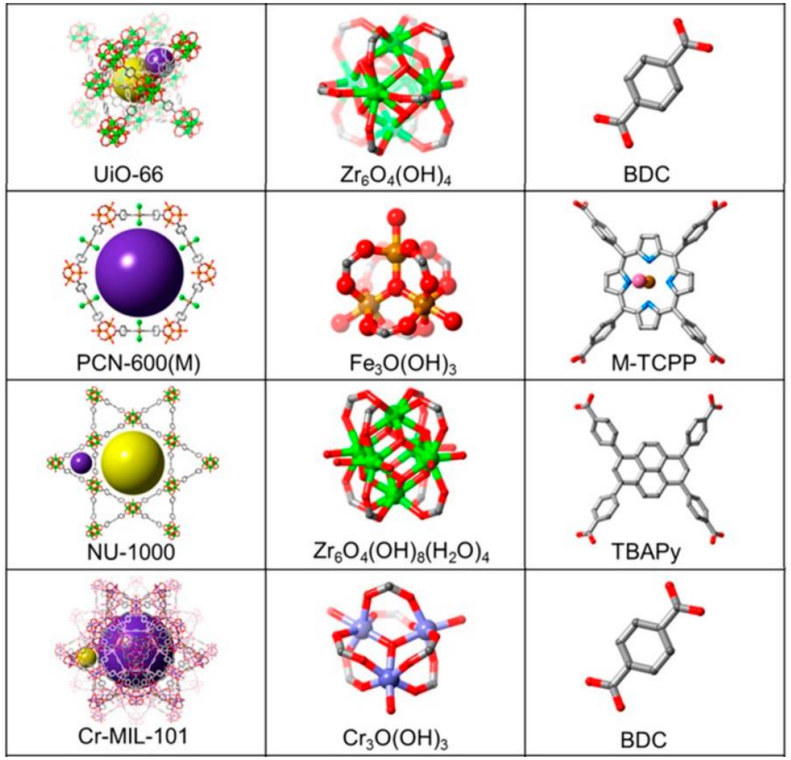
MOST-H_2 approach

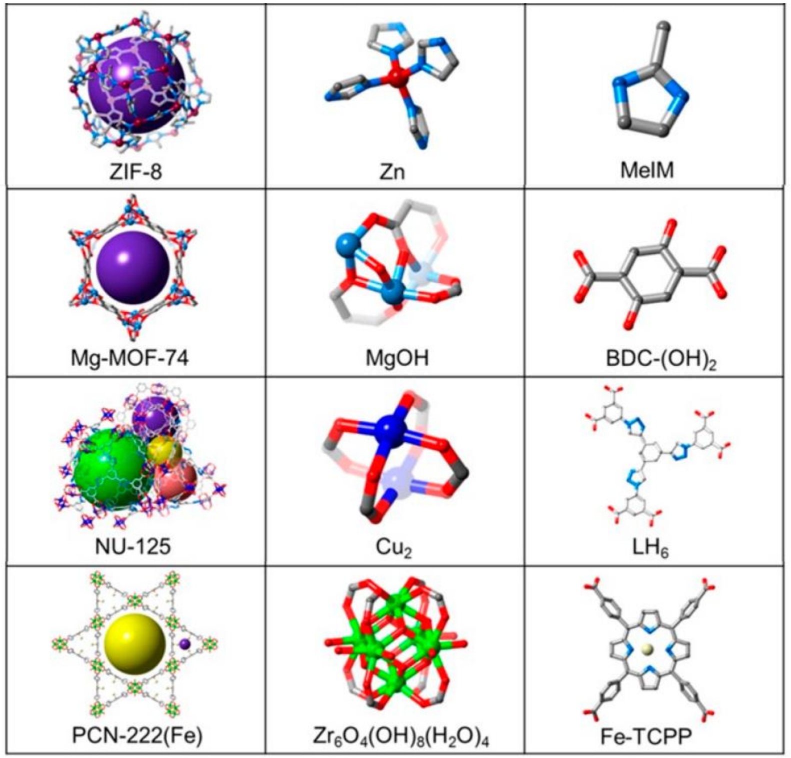


Challenge 1: How to choose the best structure

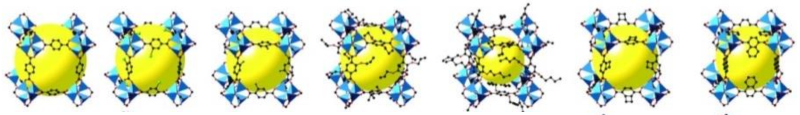
MOF structural-chemical variations



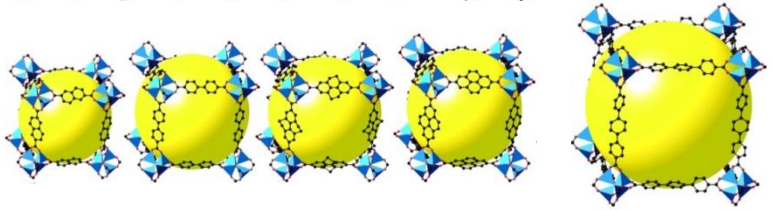
Combine



Functionalize



Expand



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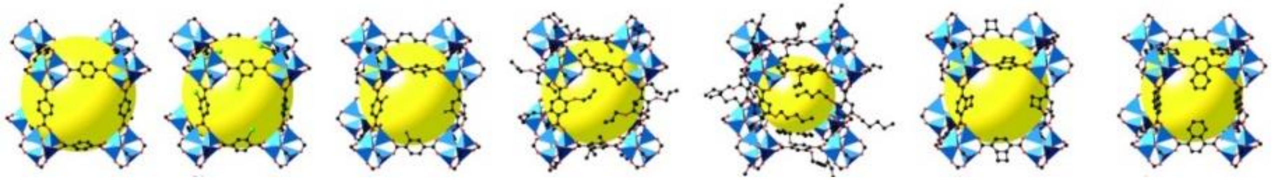
Challenge 1: How to choose the best structure

Functionalize



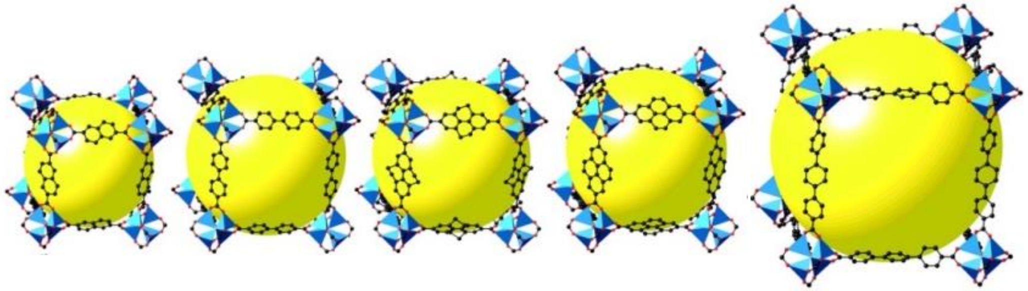
Add functionalities

Increase gas-solid interactions

Increase weight

Decrease available space (pore volume)

Expand



Stronger interactions but
not enough space (pore volume).
High volumetric-Low gravimetric

Increased surface area
but a lot of **empty space**.
High gravimetric-Low volumetric

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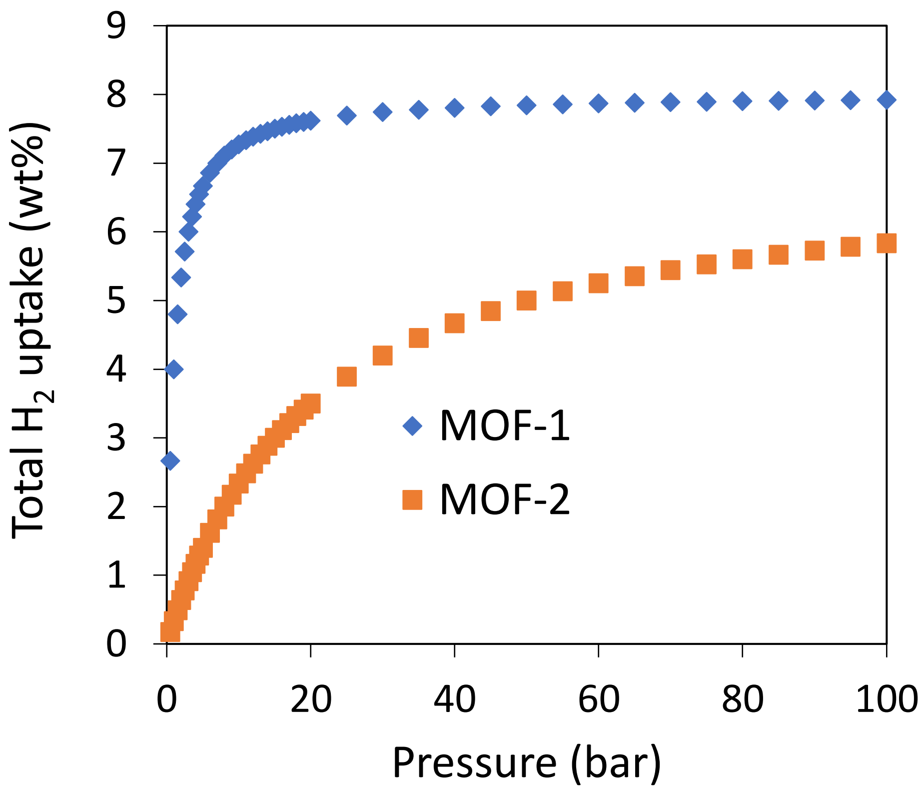
Simply maximize H_2 storage capacity?

✓ Adsorption isotherms



MOF-1 > MOF-2

✓ Routinely @ 77K (liquid N_2)

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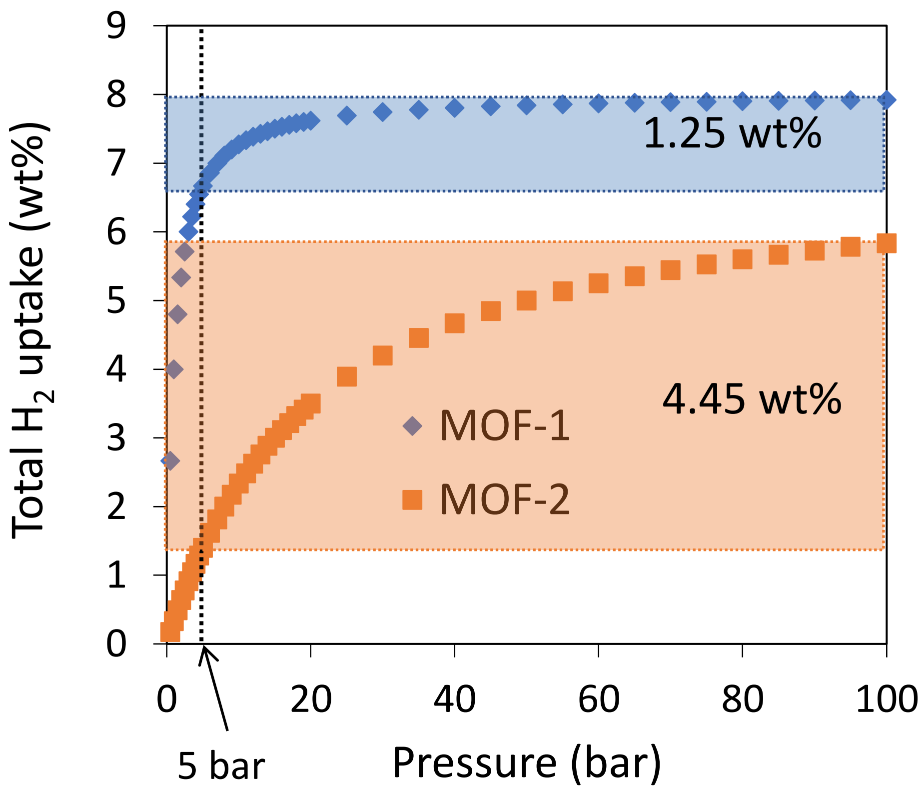
Challenge 2: Maximize H_2 deliverable capacity

✓ Uptake @ 100 bar - Uptake @ 5 bar



MOF-1 < MOF-2

✓ @ 77K (liquid N_2)

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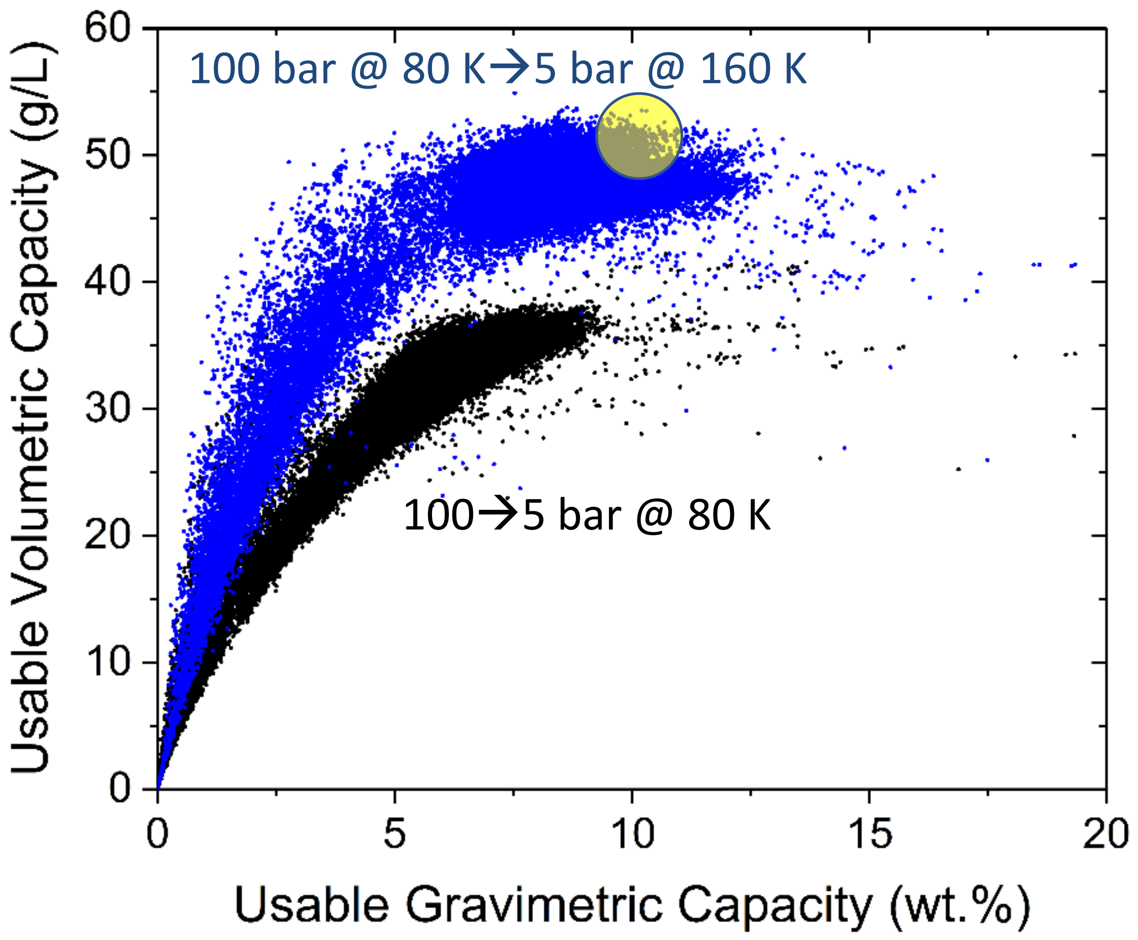
Challenges 1, 2 → ML Gravimetric & Volumetric Capacities



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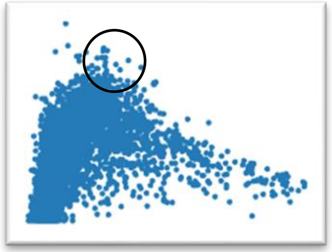
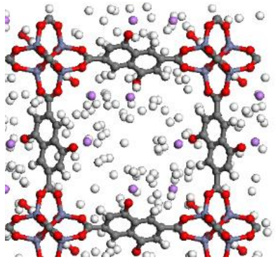
Challenges 1, 2 → ML screening MOST-H2 database

1. MOST-H2 Database Construction ($>10^4$ entries)

→

ML Screening MOST-H2 Database

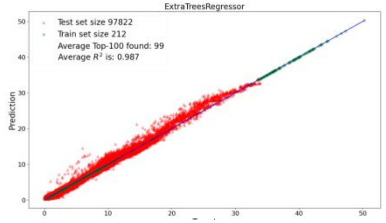


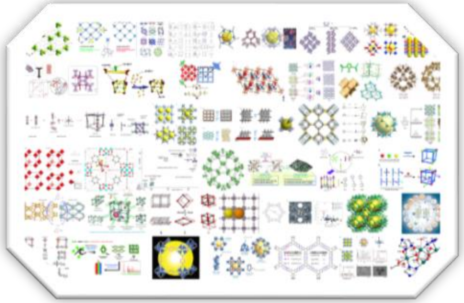


2. High throughput GCMC simulations CORE and HyMARC Databases

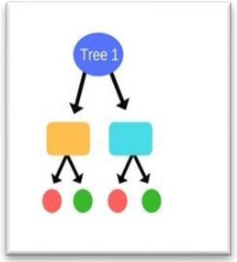
→

ML-Algorithm Training





3. ML-Algorithm Development



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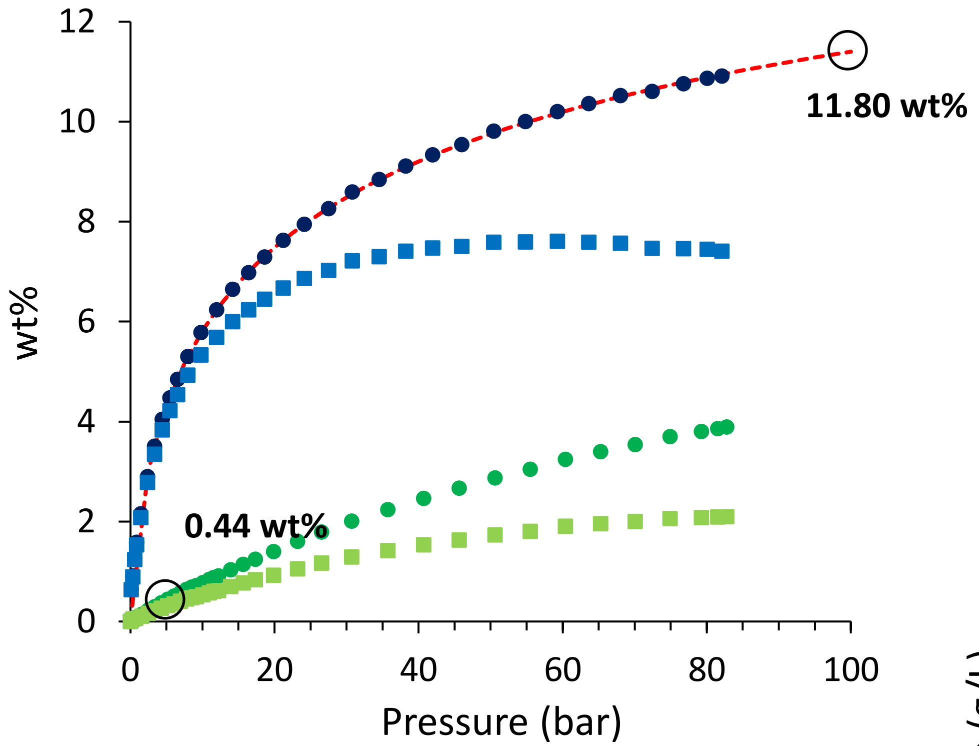
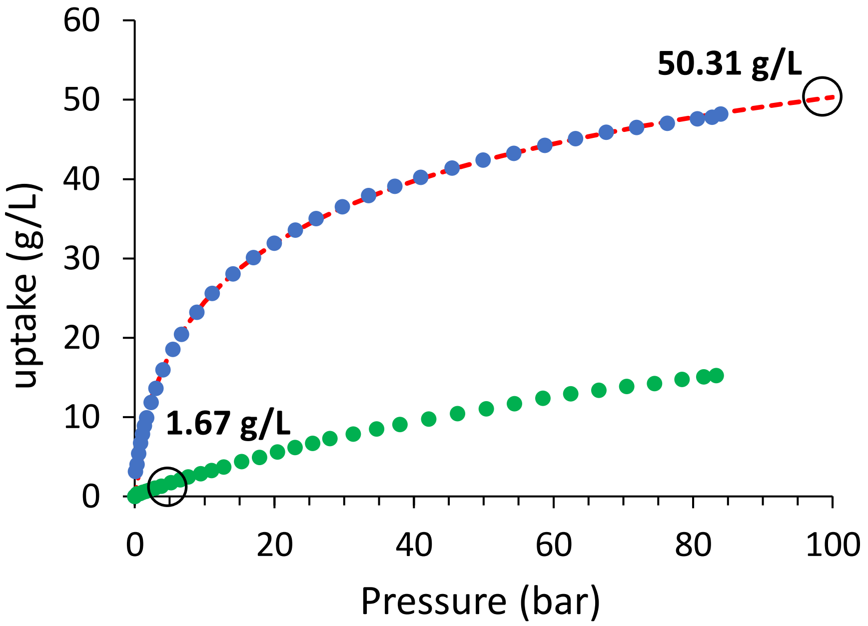
Challenges 1, 2 → Real Samples



Total usable capacity

(100 bar, 77K → 5 bar, 160K)

- 11.36 wt%
- 48.64 g/L



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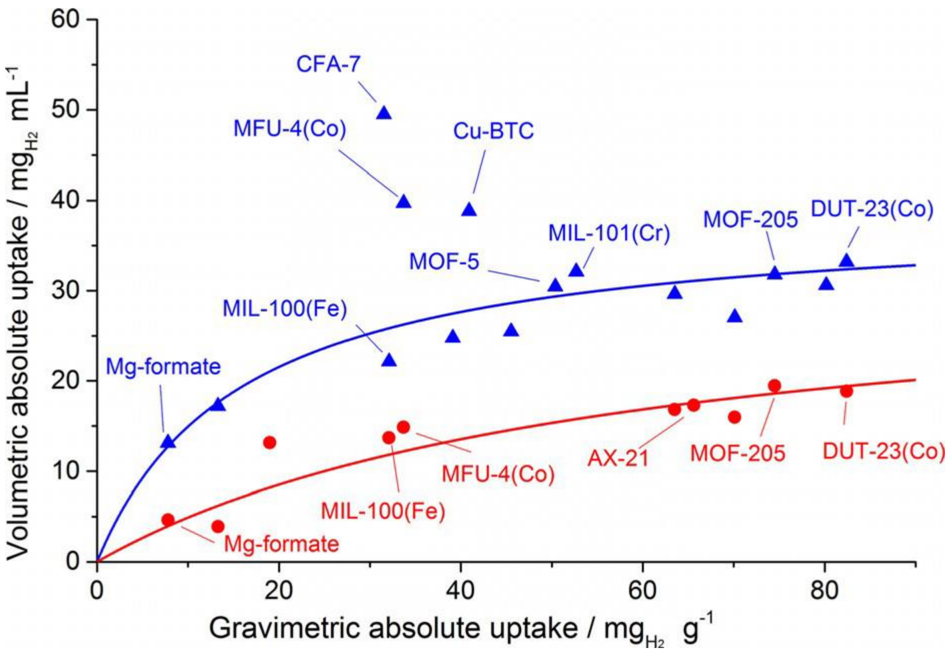
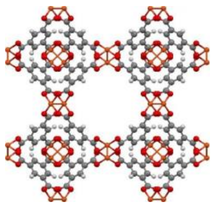
Challenge 3: Shape engineering → powder vs monolith





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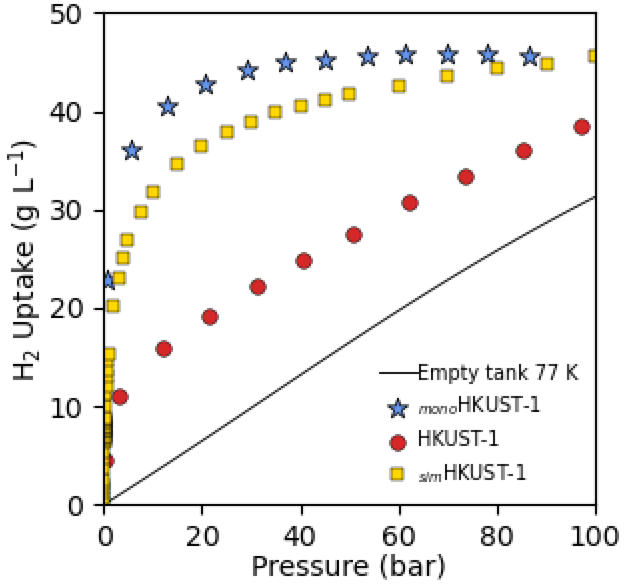
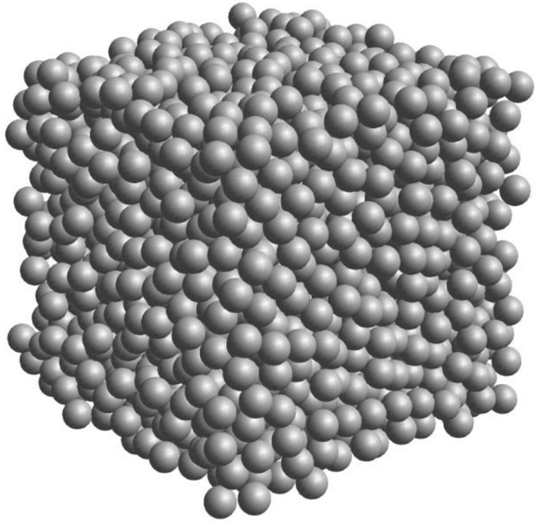
immaterial



Challenge 4: Tank packing/Heat management



$V_{MOF} / V_{tank} = 0.99$

$S\downarrow\downarrow, D\downarrow\downarrow, \lambda\downarrow$

$V_{MOF} / V_{tank} < 0.65,$

$S\uparrow\uparrow, D\uparrow\uparrow, \lambda\downarrow\downarrow$

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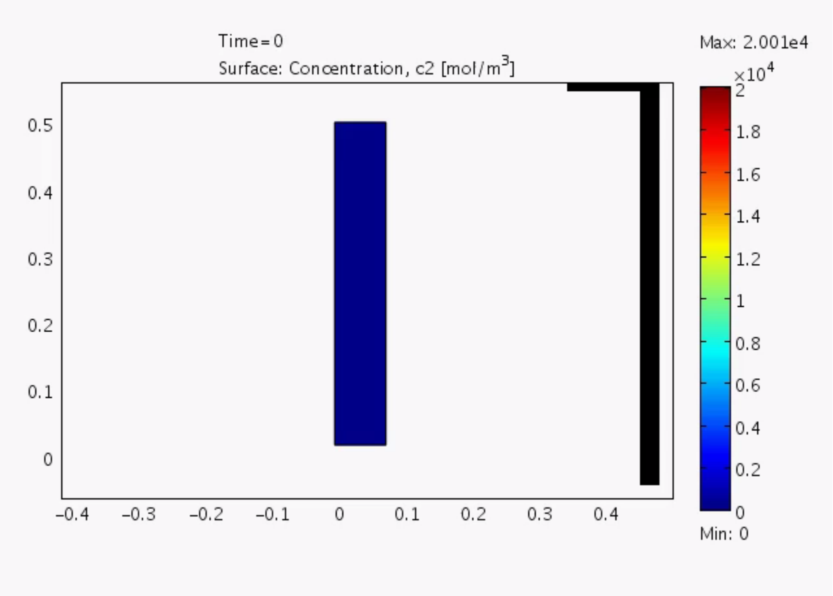
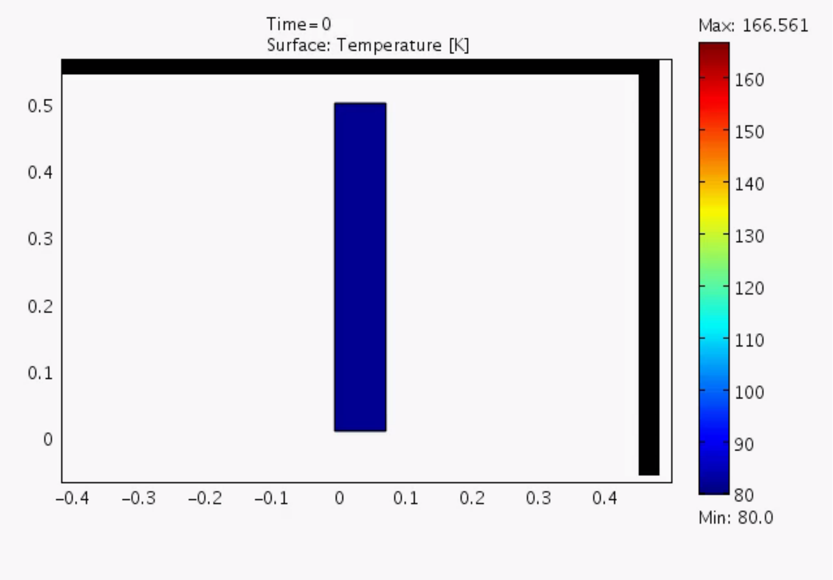
Challenge 4: Tank design/modelling

Concentration



Temperature



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Technology validation/assessment

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Tank testing

Hydrogen Refuelling Station for small vehicles installed at the premises of NCSR DEMOKRITOS

GreenDelta

Performance data

Full Life Cycle Sustainability Assessment of the new adsorbents

Techno-Economic Analysis of using MOF-based H_2 storage systems in stationary & rail / road applications

fen research

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