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Integrating process design and materials genomics for energy efficient adsorption-based capture technologies

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AIChE Annual Meeting

17 November 2020

The Background to the Problem

Preliminary efforts

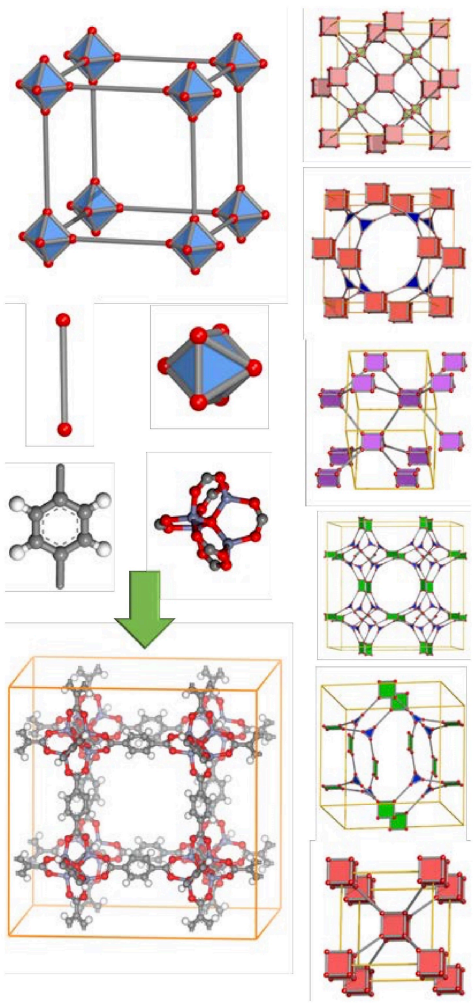
The innovation in PrISMa

PrISMa Workflow

Some examples

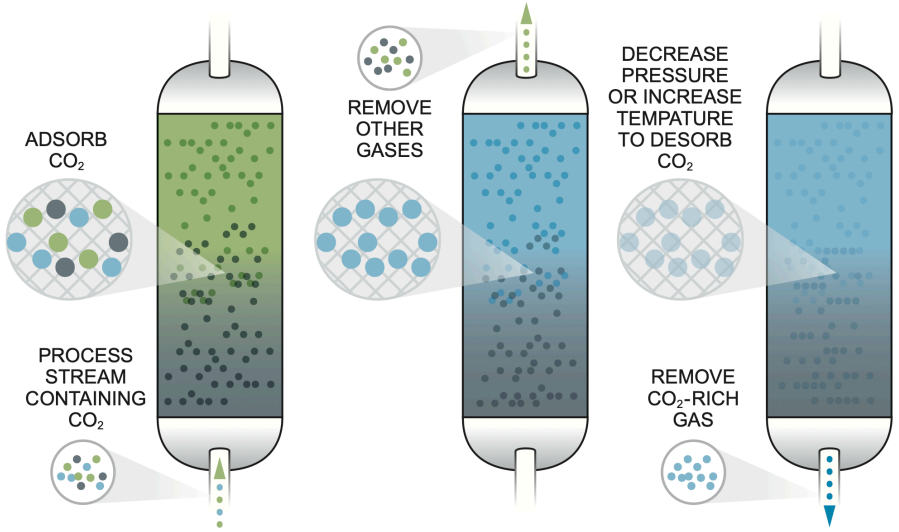
MatScreen: Our automated screening platform

The Background to the Problem

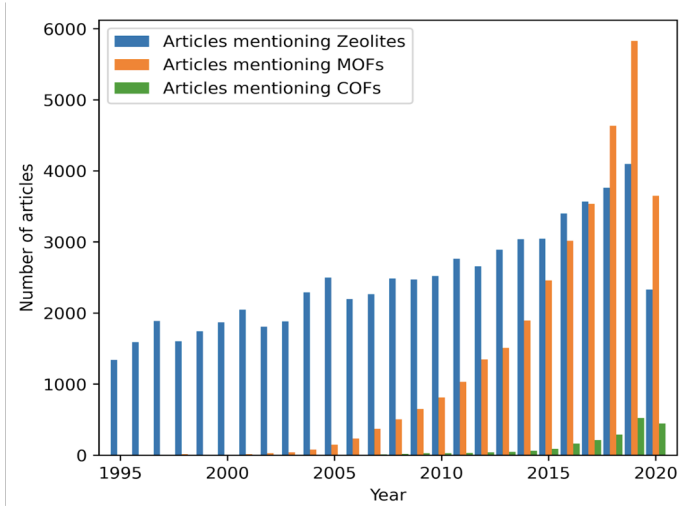


The Challenge:

"There is currently no ability to quickly identify what processes and process conditions are optimal for a particular adsorbent to achieve the required specifications for a capture application" (Mission Innovation report)[1]



CO_2 capture by Adsorption. Source: CO2CRC



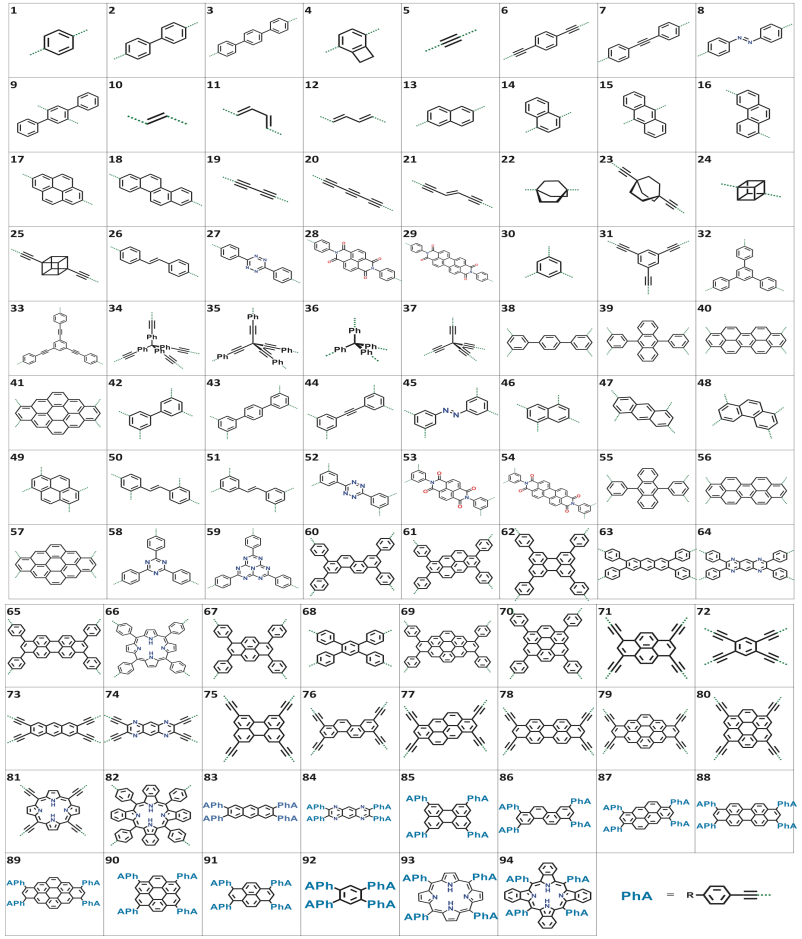
- For maximum impact of breakthrough materials, ***processes and materials must be developed hand-in-hand*** for any particular application.
- The ***integration between molecular science and process engineering*** is a significant gap of knowledge which hinders the realization of many novel promising materials beyond lab scale testing.

[1] Carbon Capture, Utilization and Storage Expert's Workshop (2017) *Accelerating Breakthrough Innovation in Carbon Capture, Utilization, and Storage*. Houston, Texas.

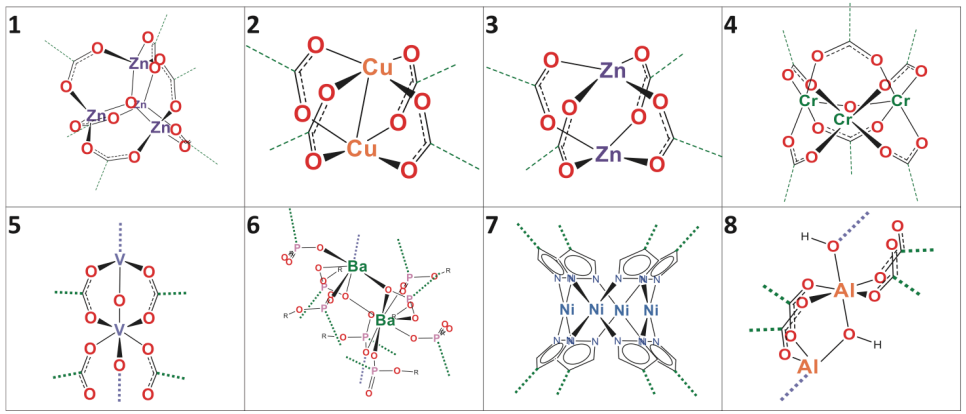
Our previous efforts

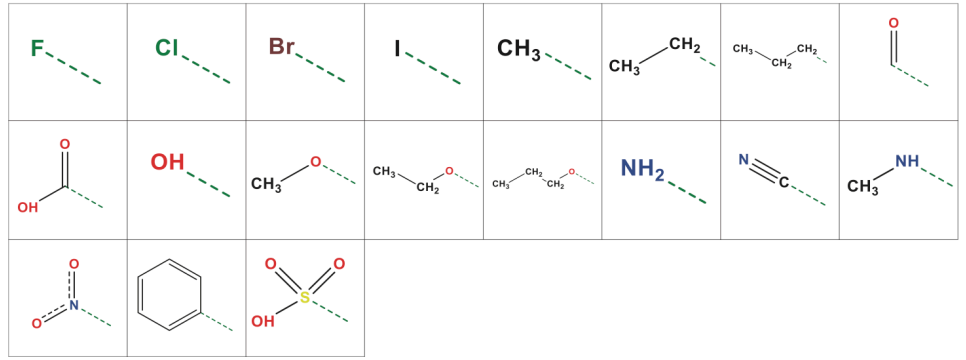
What's the best MOF material for wet flue gas CO_2 capture?

In-silico screening



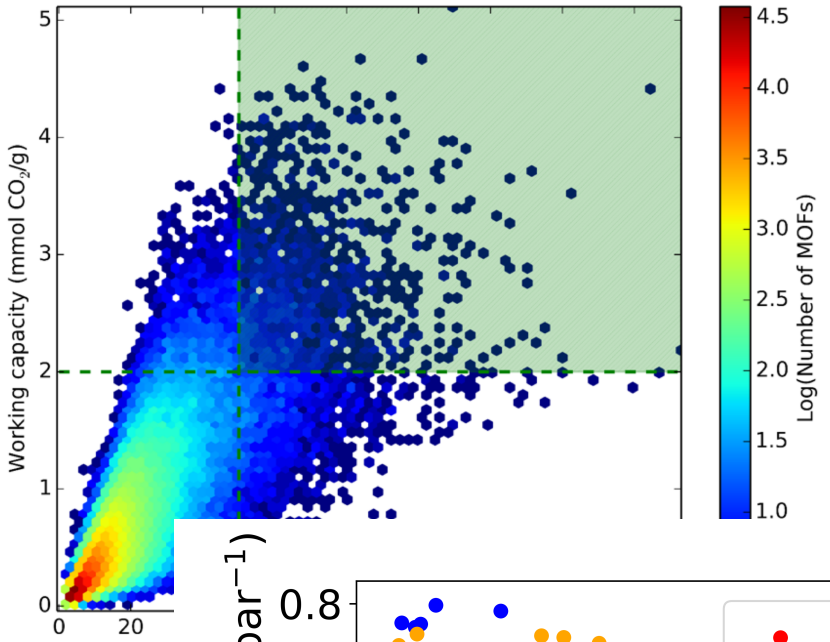
Total: 325,000 MOFs

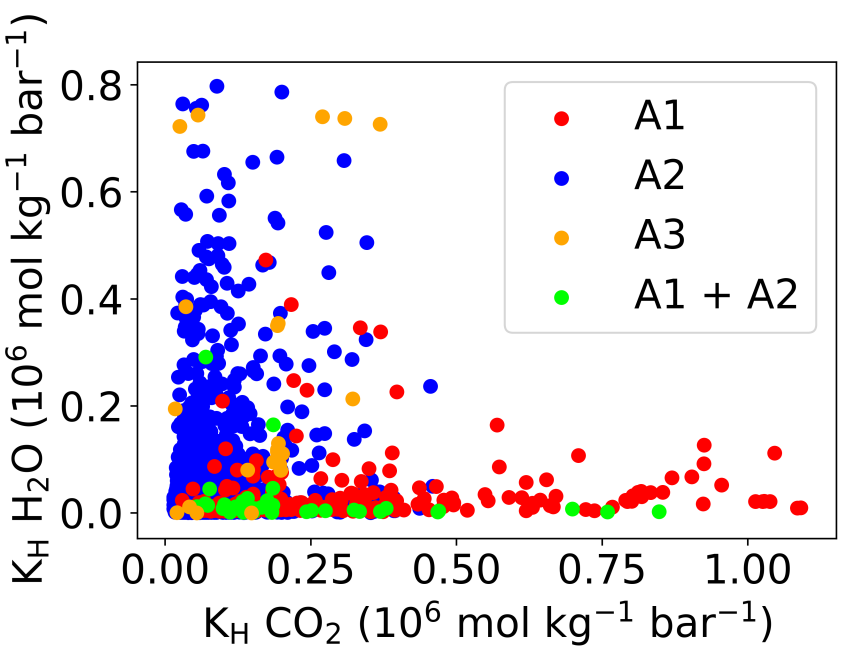




Boyd, P.G., Chidambaram, A., García-Díez, E. *et al. "Data-driven design of metal–organic frameworks for wet flue gas CO_2 capture".* ***Nature*** **576,** 253–256 (2019). https://doi.org/10.1038/s41586-019-1798-7

The Adsorbaphore concept

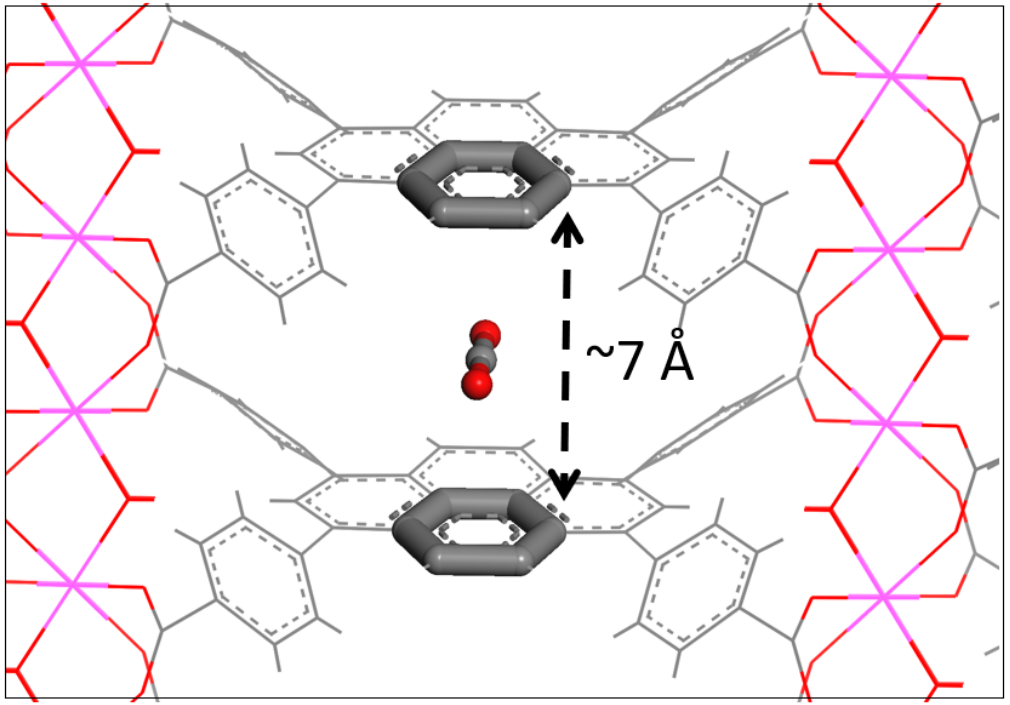




Adsorbaphore (pharmacophore):

- Two parallel aromatic rings with interatomic spacing of approximately 7 Å (31% of all binding sites)
- Metal–oxygen–metal bridges (32%)
- Open metal sites (21%)

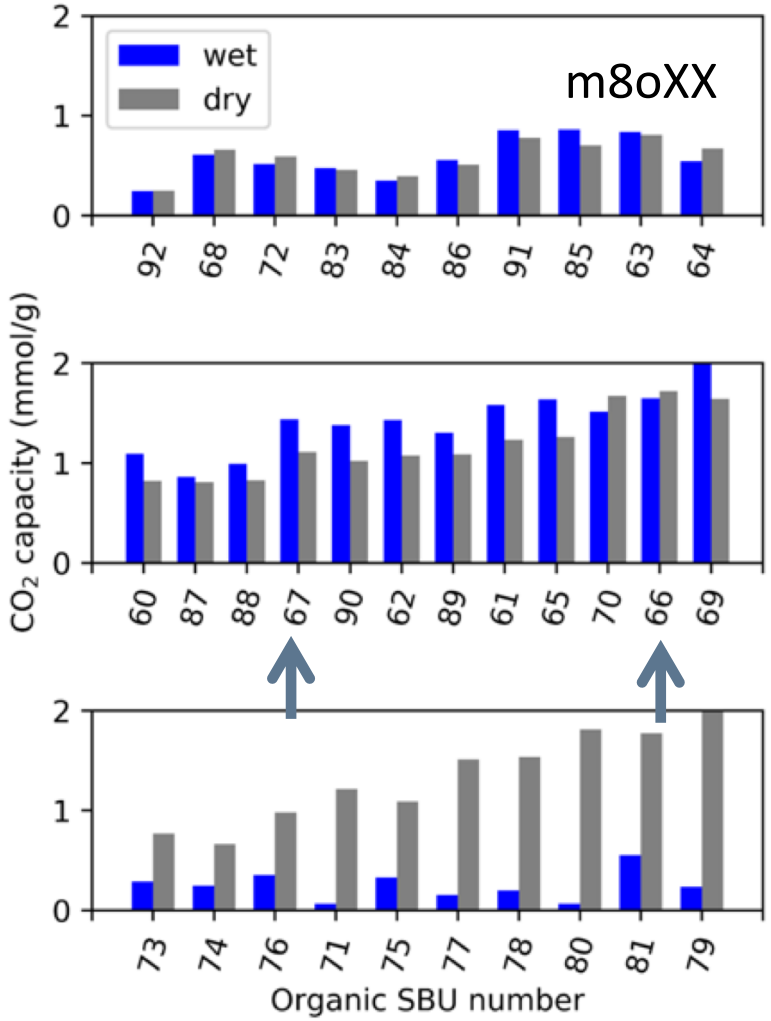
The parallel aromatic rings adsorbaphore discovered with the feature recognition algorithm.



The CO_2 capacity: what materials to synthesize

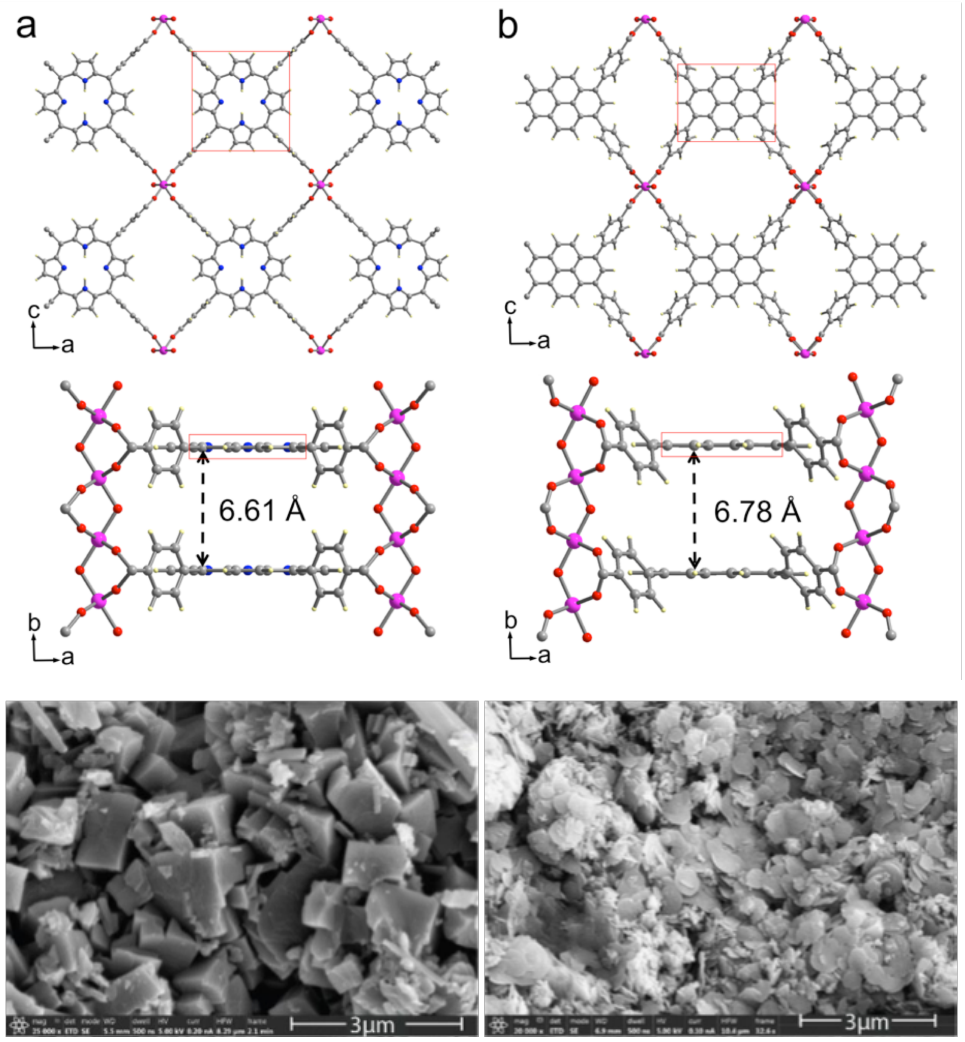
Second library using experimental input:

H_20 stable abundant MOFs (Al)



Hypothetical MOFs built with the frz topology

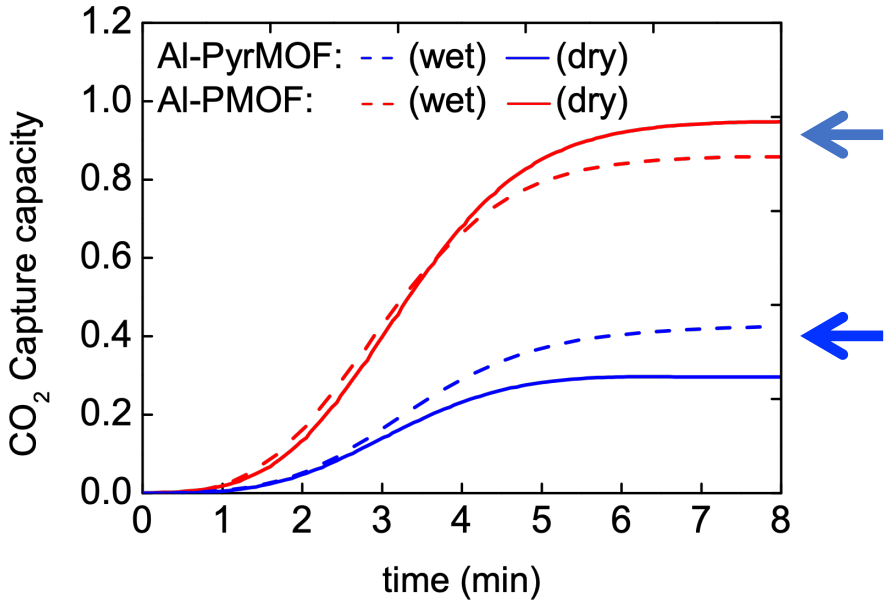
Al-PMOF **Al-PyrMOF**

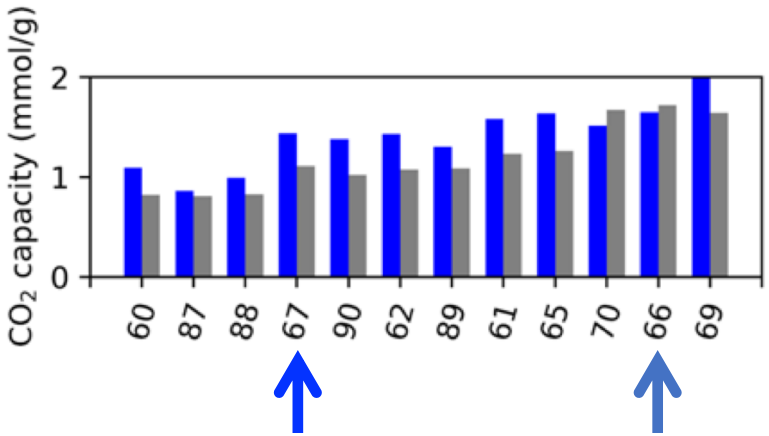


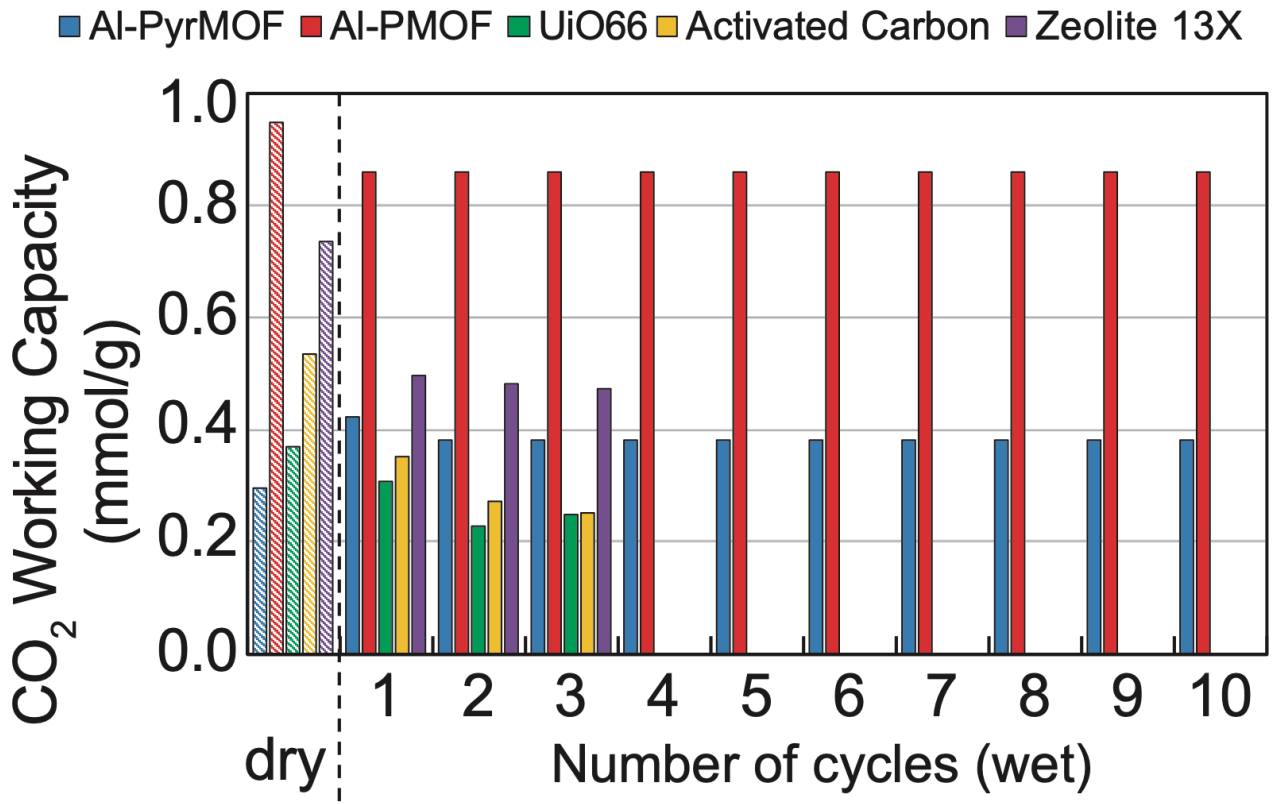
Fateeva *et al*, Angew. Chem.-Int. Edit. 2012, **51**, 7440.

Process Performance and Benchmarking

Mixture: N_2/CO_2 (+water)





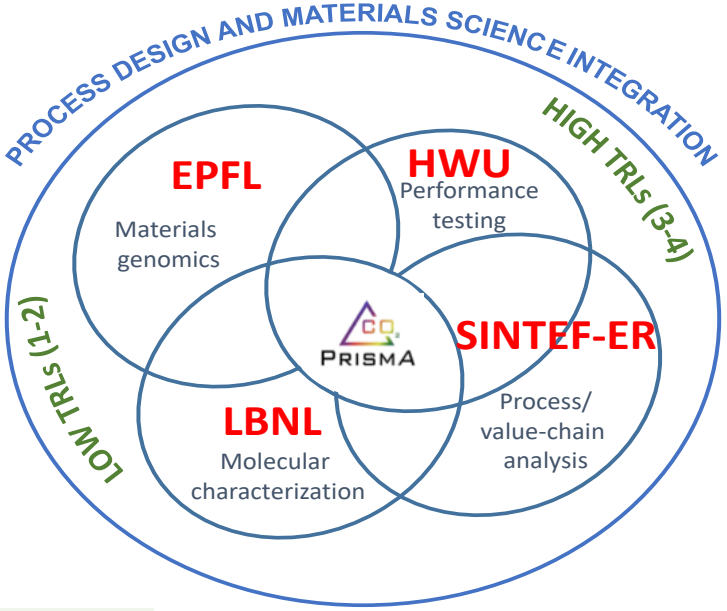


BUT WE WANTED TO DO BETTER…

The PrISMa Project

PrISMa: Process-**I**nformed design of tailor-made **S**orbent **Ma**terials for energy efficient carbon capture

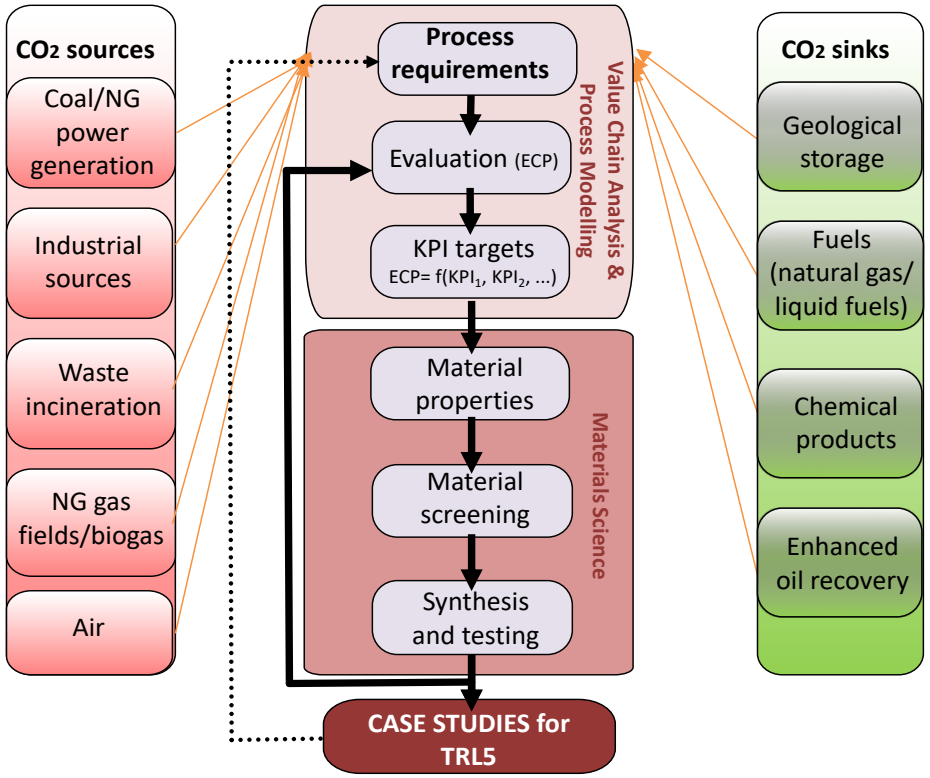
Aim: To accelerate the transition of energy and industrial sectors to a low-carbon economy by developing a technology platform to tailor-make cost-efficient carbon capture solutions for a range of different CO_2 sources and CO_2 use/destinations.



Accelerating CCS Technologies

ACT-Funded Project
€2.9M, 4 Research partners and 13 Industrial Partners
Duration: 3 years (Sept19-Aug22)

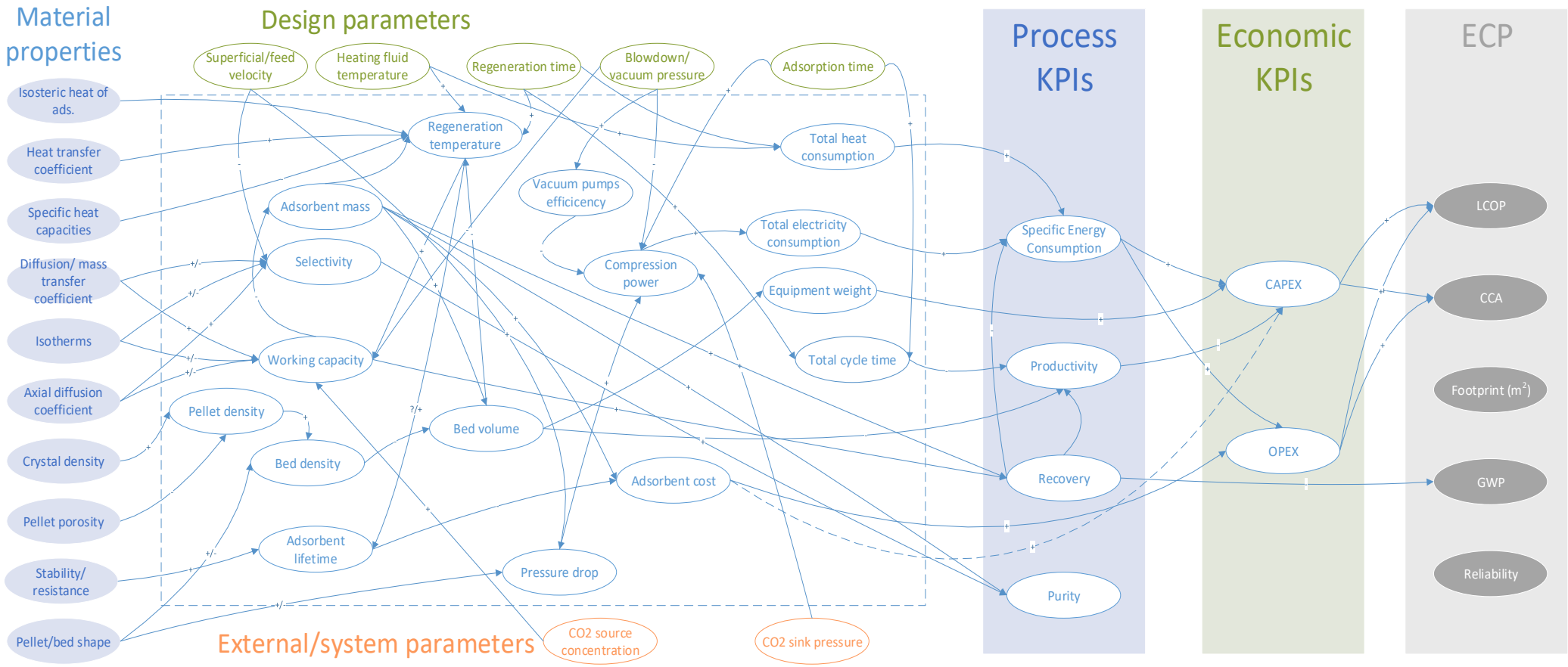
The PrISMa Platform



Key Technical Outputs

- ✓ A **technology platform** that allows us to identify for a given source and target of CO_2 the optimal capture technology. This platform is based on a ***methodology for systematic knowledge exchange between material science and process engineering***.
- ✓ A **set of case studies**, inspired by the interest of the national funding agencies and our industrial advisory board, ***to bring the technology/material to the TRL5 level***.

Cause and Effect Diagram for the Screening Methodology



How to link material properties with Process KPIs, Economic KPIs and ECP

The Screening Workflow

Case Study

CO_2 source/sink characteristics

Molecular Simulation

physicochemical + adsorptive properties

Parameters for Optimization

set a range to the process parameters

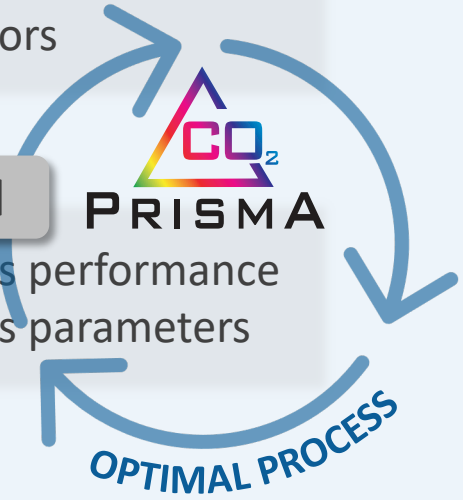
Optimization Tool

Process Models

- process performance evaluation
- process indicators

Optimization Tool

- optimal process performance
- optimal process parameters



Material Ranking

rank thousands of adsorbents based on process indicators

Material Properties

- target ranges of key parameters
- optimal material characteristics

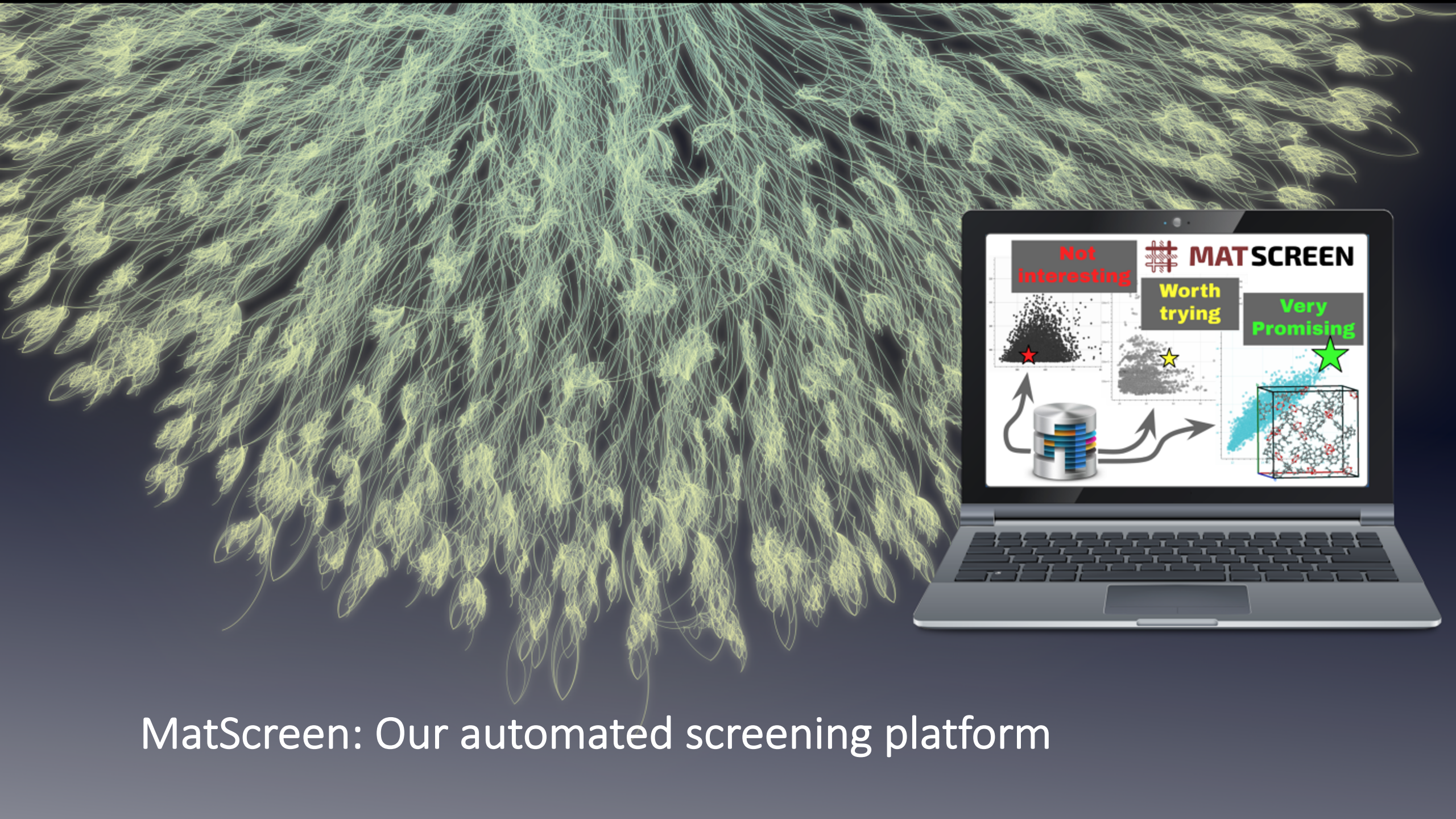
Some Examples of ongoing work in PrISMa

Charithea Charalambous is Speaking at the
2020 Virtual AIChE® Annual Meeting

CO2 Capture By Adsorption II

CO2 Recovery from Ultra-Dilute Streams: Bridging a Novel Temperature Vacuum Swing Adsorption Model with Materials Screening

Date: Thursday, Nov 19 8:00 AM

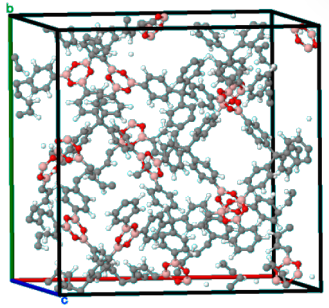


MatScreen: Our automated screening platform

An Automated Framework from Crystal structure to Carbon Capture

Data refinement

Checking:
- atoms overlapping
- missing H
- chemistry
- solvent

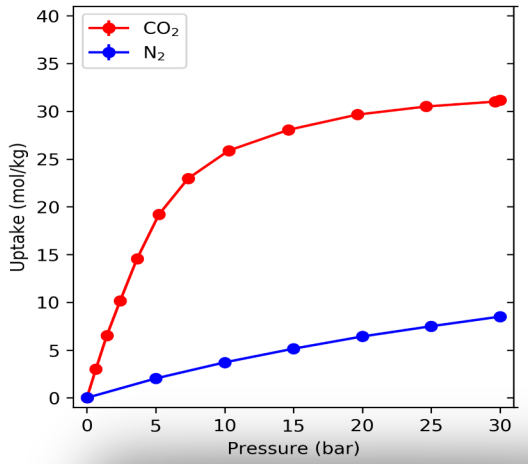


Geometry optimization

CP2K
- checking stability
- reliable optimum cell & geometry
- partial charges

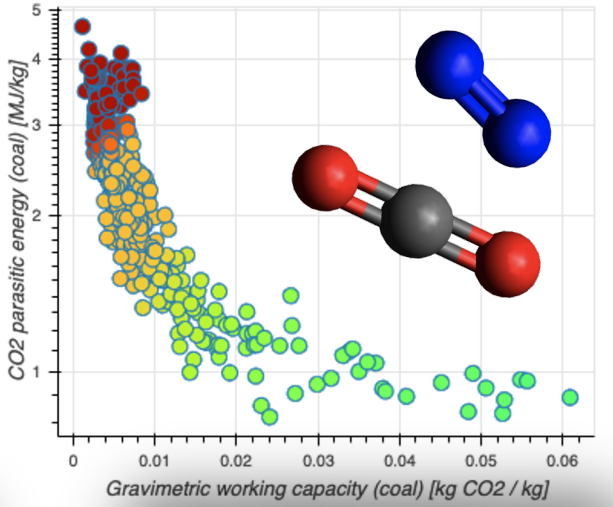
Geometry characterization

Zeo++
- PLD, LFS
- surface / pore vol.
- blocking spheres



Adsorption properties

RASPA
For CO_2 and N_2:
- Henry coefficient
- Adsorption isotherm
- Heat of adsorption



Process modelling

calPE.py
- parasitic energy
  kJ/kg[CO_2]
- optimal T/P desorption
- working capacity
- final CO_2 purity

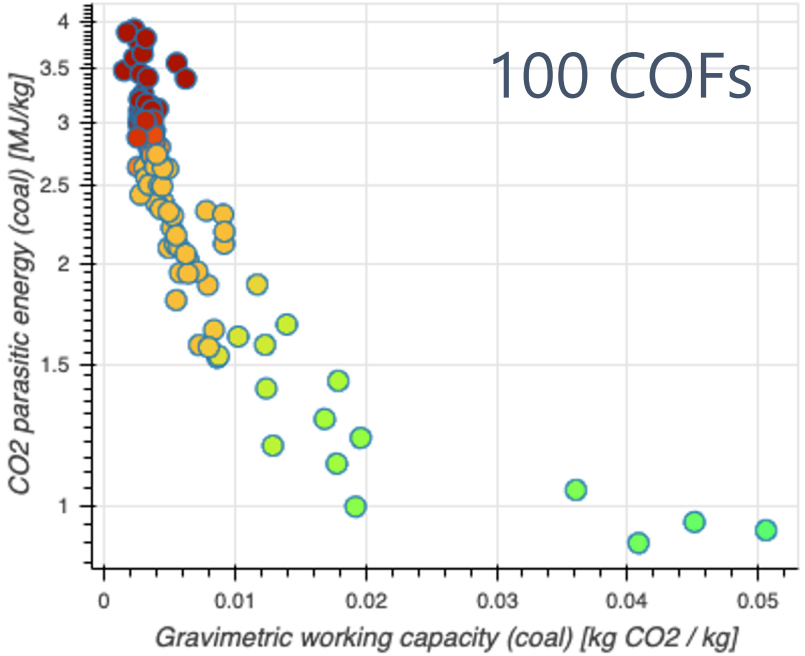
D. Ongari, A.V. Yakutovich, L. Talirz, B. Smit, *Building a consistent and reproducible database for adsorption evaluation in COFs*, ACS Cent. Sci. 2019

D. Ongari, L. Talirz and B. Smit, *Too many Materials and too many applications: an experimental problem waiting for a computational solution*, ACS Cent. Sci. https://dx.doi.org/10.1021/acscentsci.0c00988

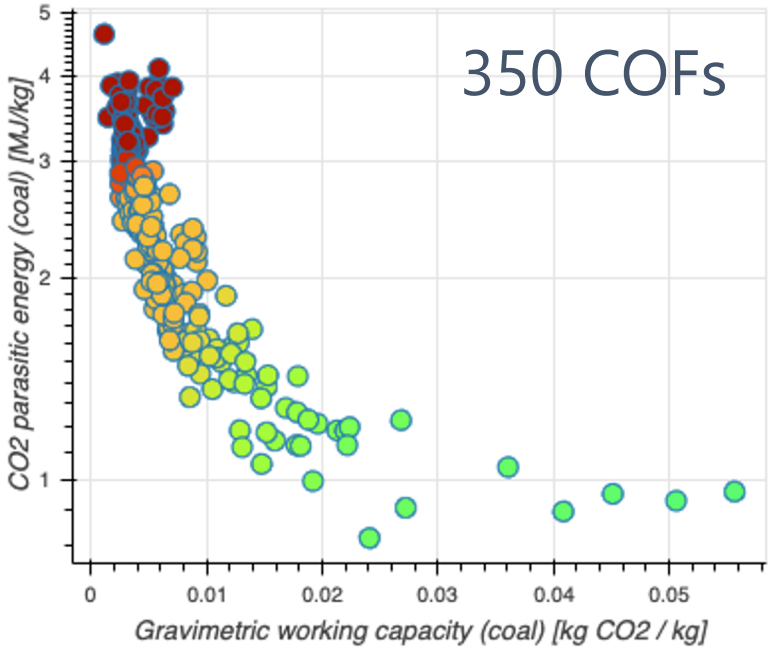
Case Study- COFs for CO_2 capture: Updates and Surprises

PRISMA

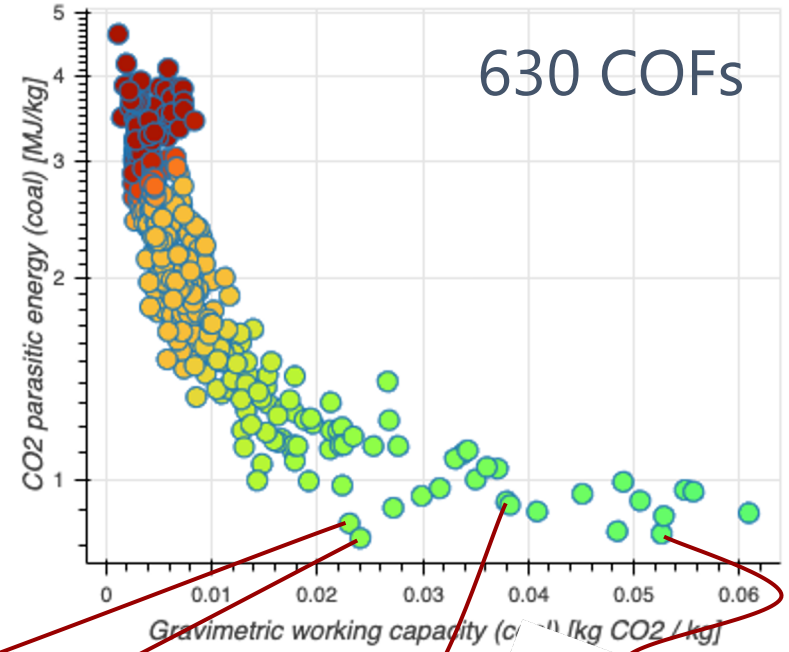
2007 - 2014

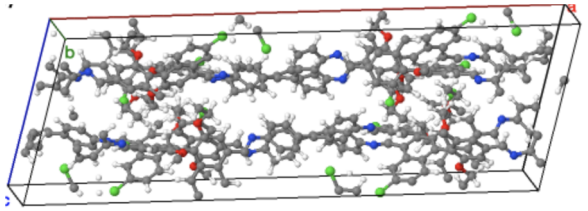


2015 - 2018

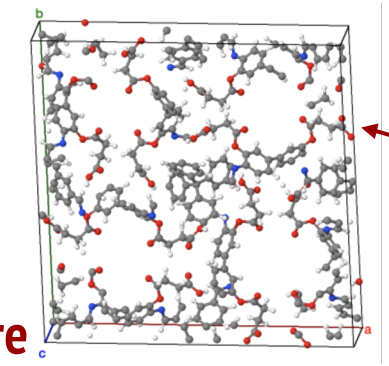


2019 - 2020



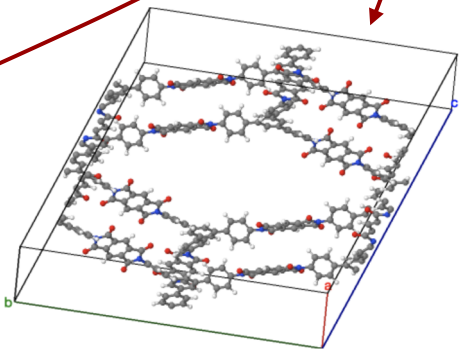


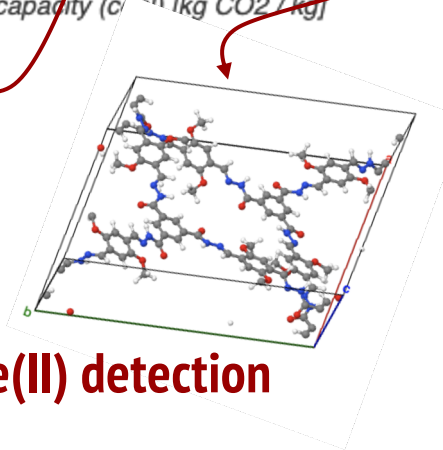
Sensing of aromatics



Ions capture

CO_2 photoreduction

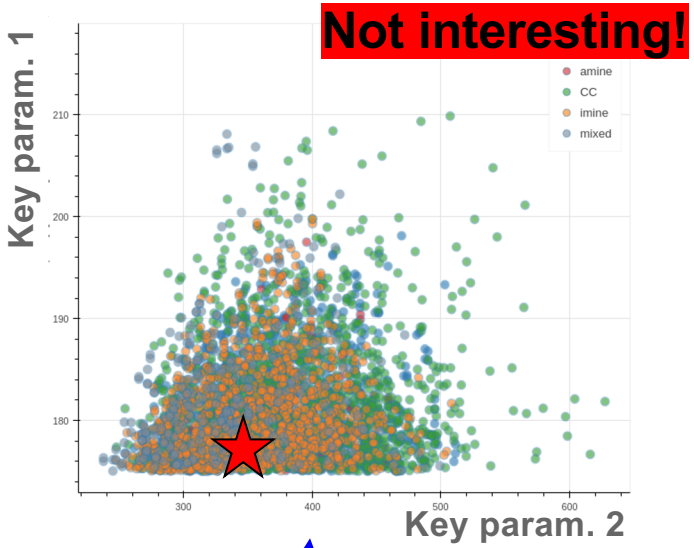




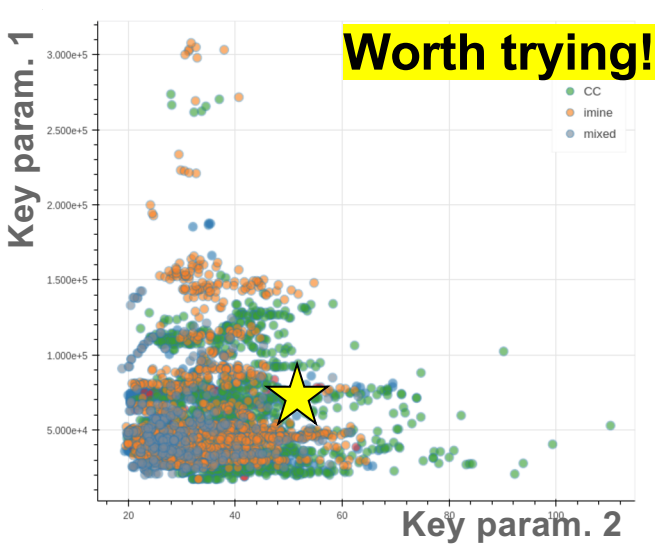
Fe(II) detection

A matching platform for materials and applications

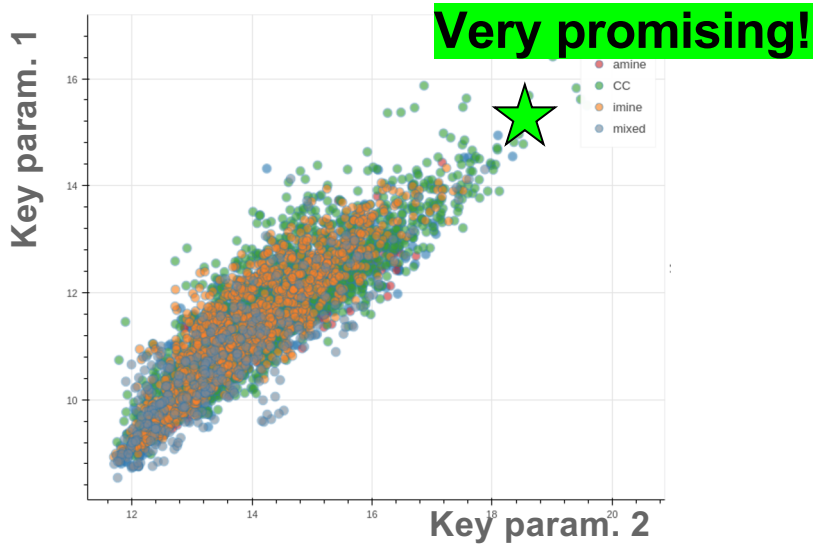
Separation #1 (source X, sink Y)

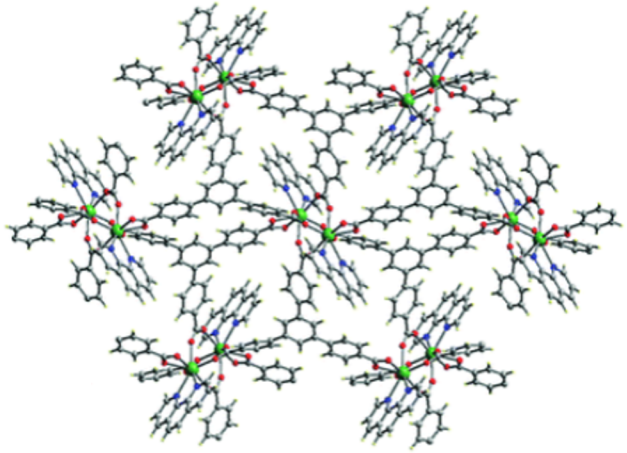


Separation #2 (source X, sink Y)



Separation #3 (source X, sink Y)





Acknowledgments

This PrISMa Project (No 299659) is funded through the ACT programme (Accelerating CCS Technologies, Horizon2020 Project No 294766). Financial contributions made from: BEIS together with extra funding from NERC and EPSRC, UK; RCN, Norway; SFOE, Switzerland and US-DOE, USA, are gratefully acknowledged. Additional financial support from TOTAL and Equinor, is also gratefully acknowledged.

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