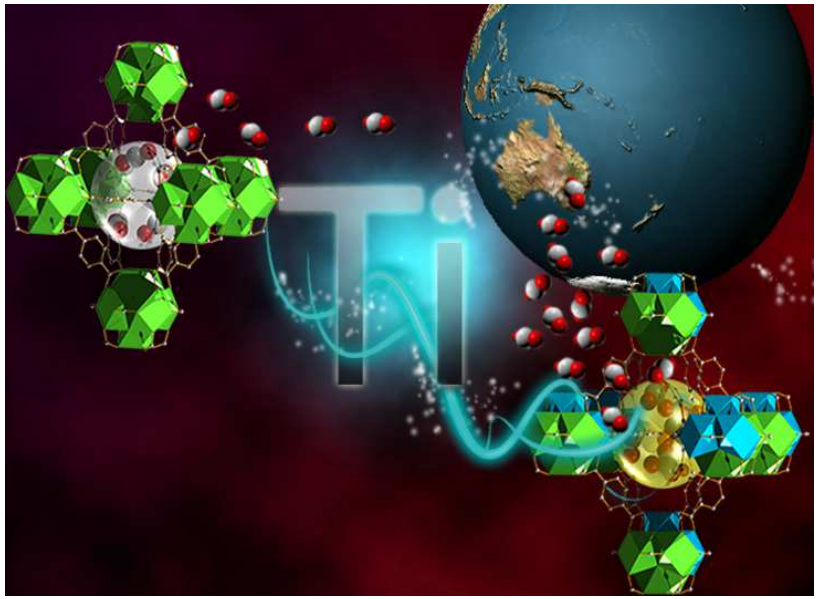
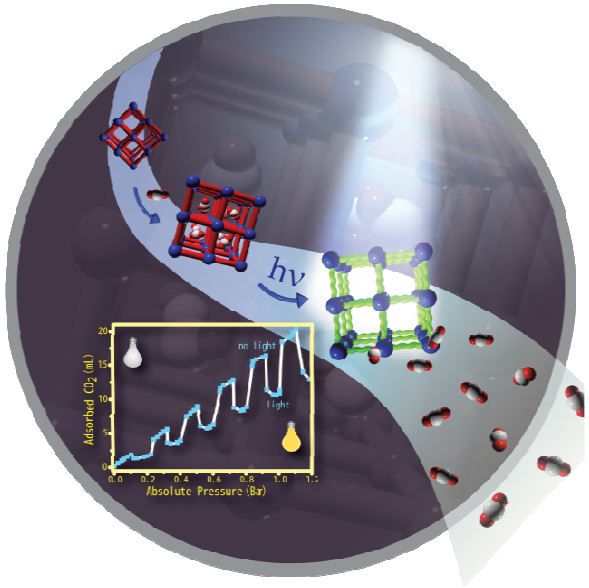




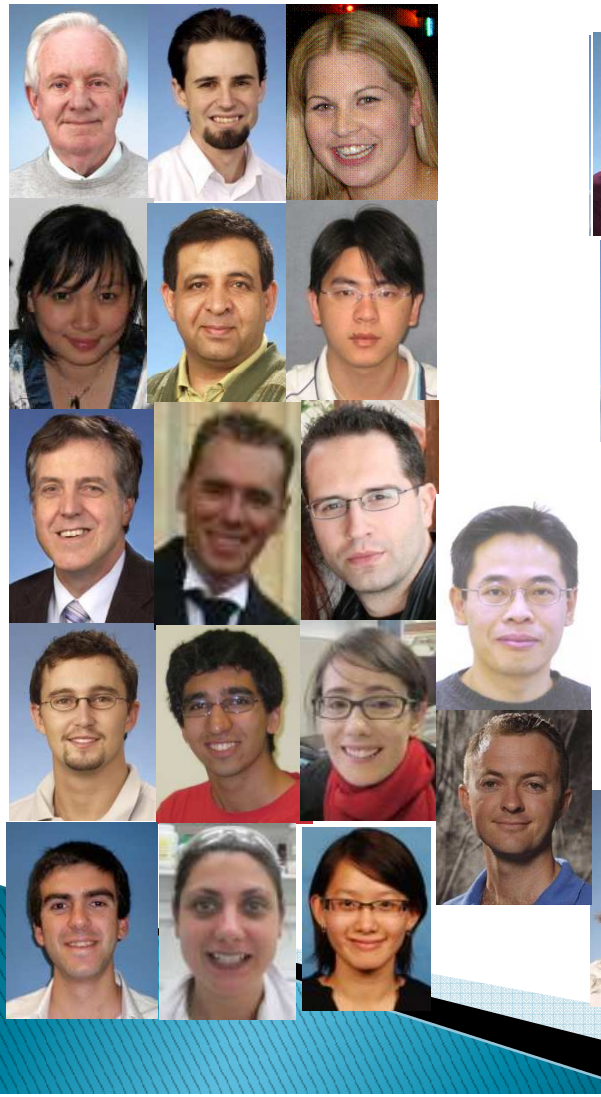
CO_2 Storage and Separation in Metal Organic Frameworks

Matthew Hill

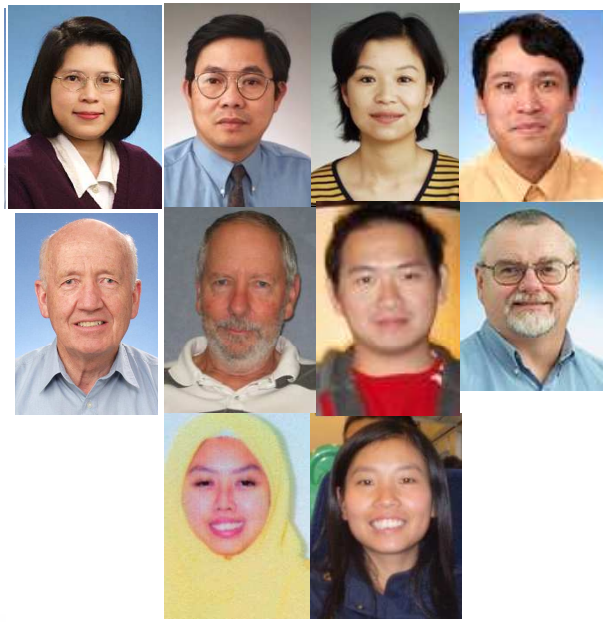
CSIRO /MATERIALS SCIENCE AND ENGINEERING

Materials for Energy, Water and Environment group

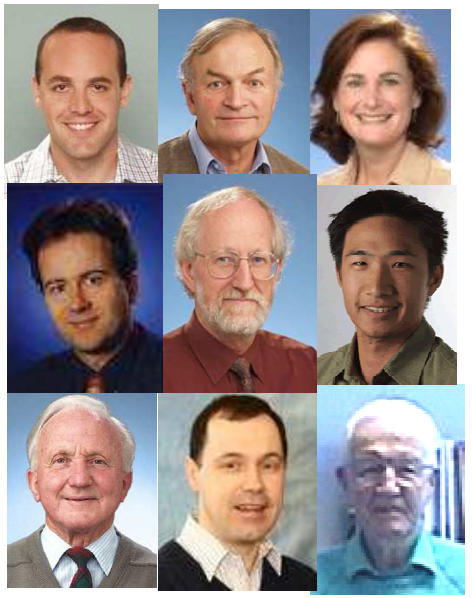
Nanoporous Materials



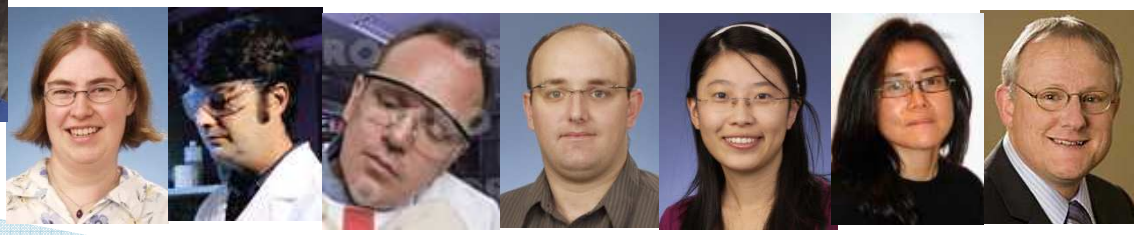
Environmental Catalysis and Membranes

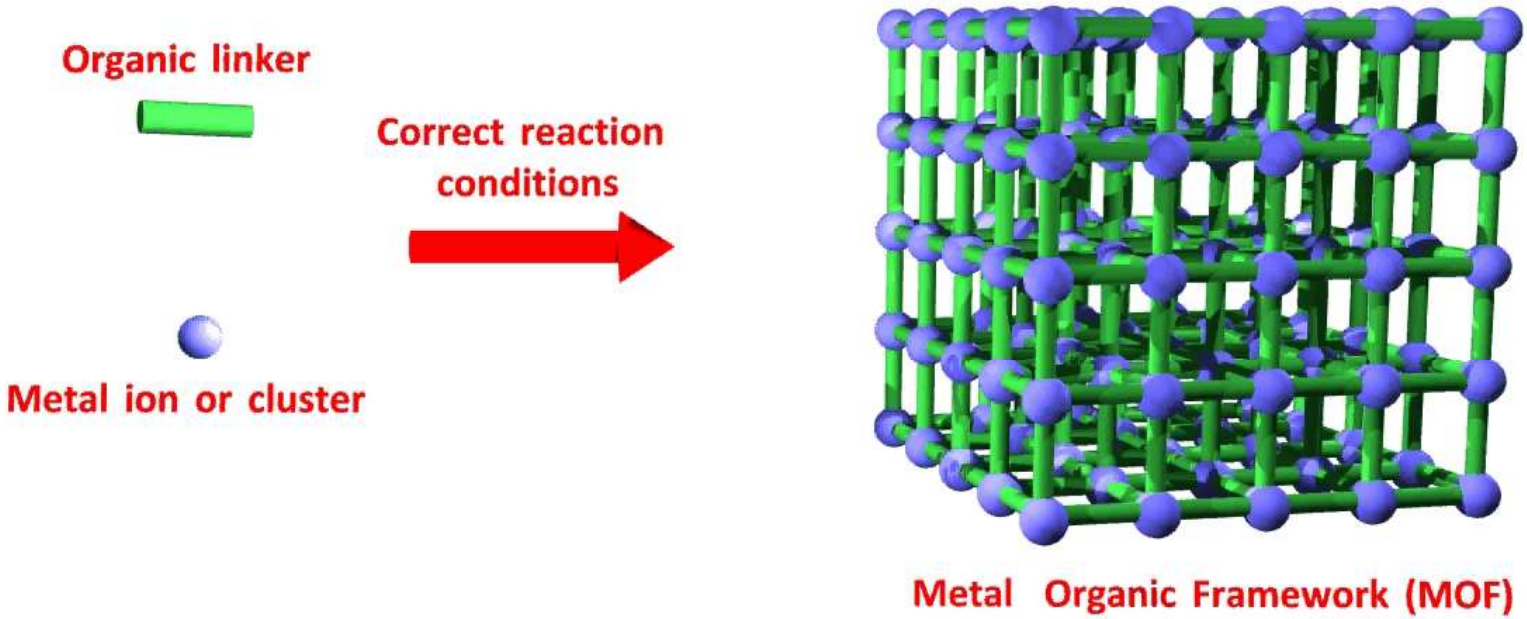


Active Nanostructures



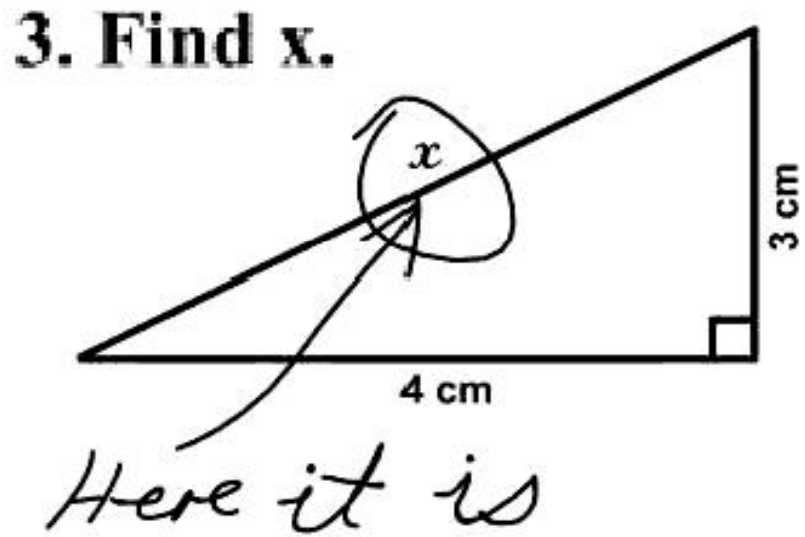
Soft Matter Chemistry and Physics



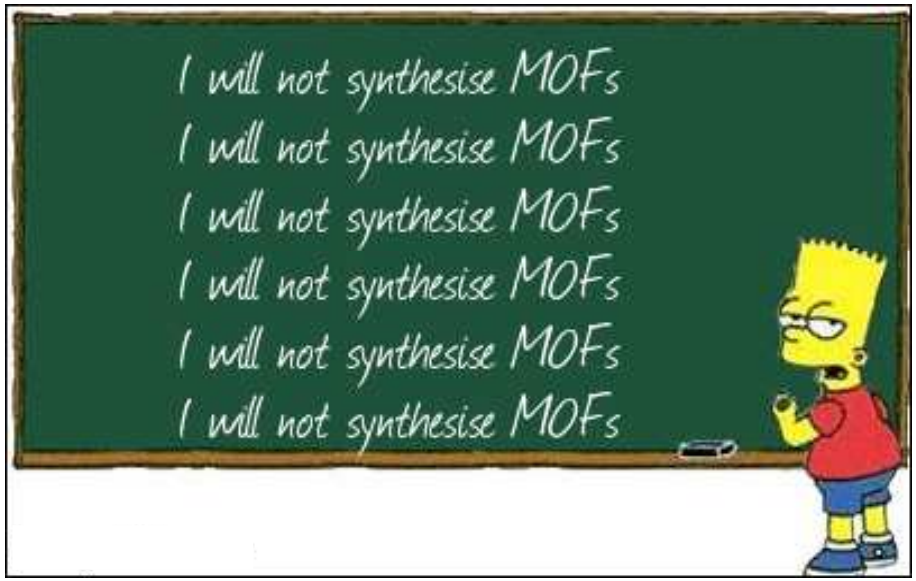


MOF synthesis is hard!!!

Geometry
(coordination chemistry)

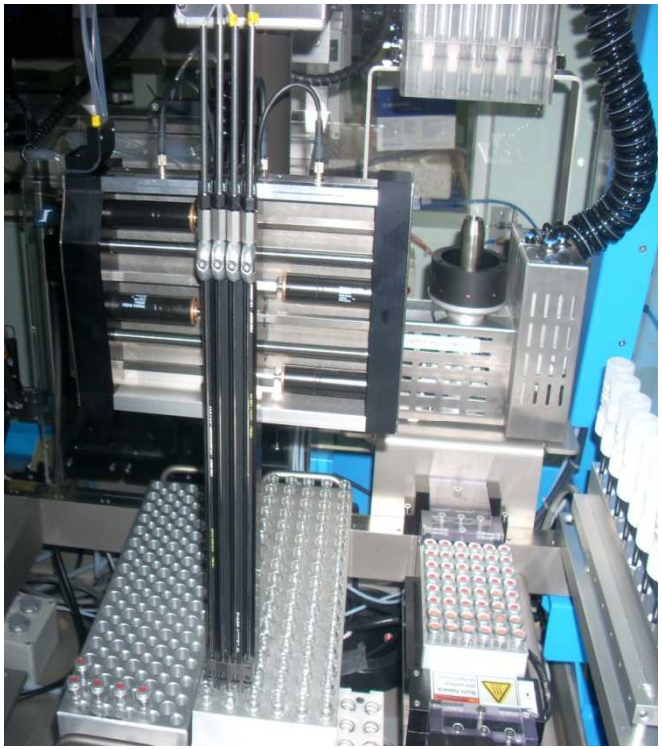


Repetition
(polymer chemistry)



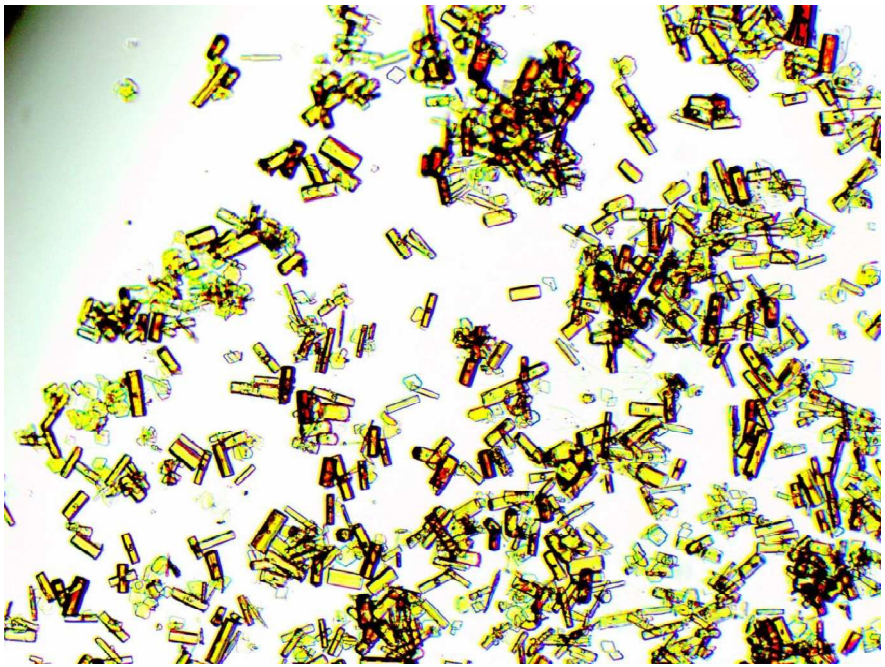
MOFs (aka Coordination polymers) require coordination chemistry + polymer chemistry simultaneously.

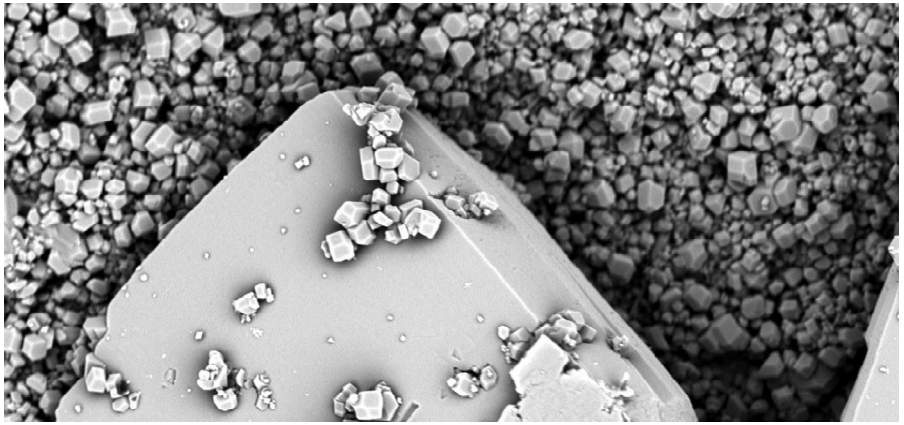
High Throughput Synthesis of MOFs



Danielle Kennedy

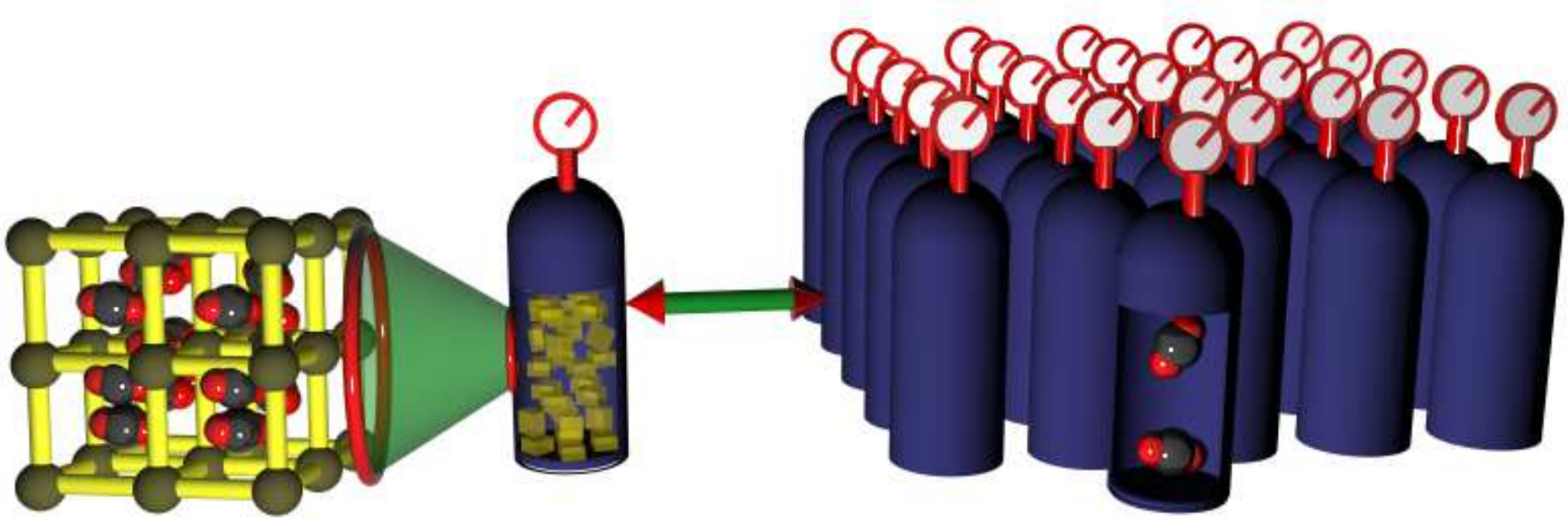
What MOFs look like



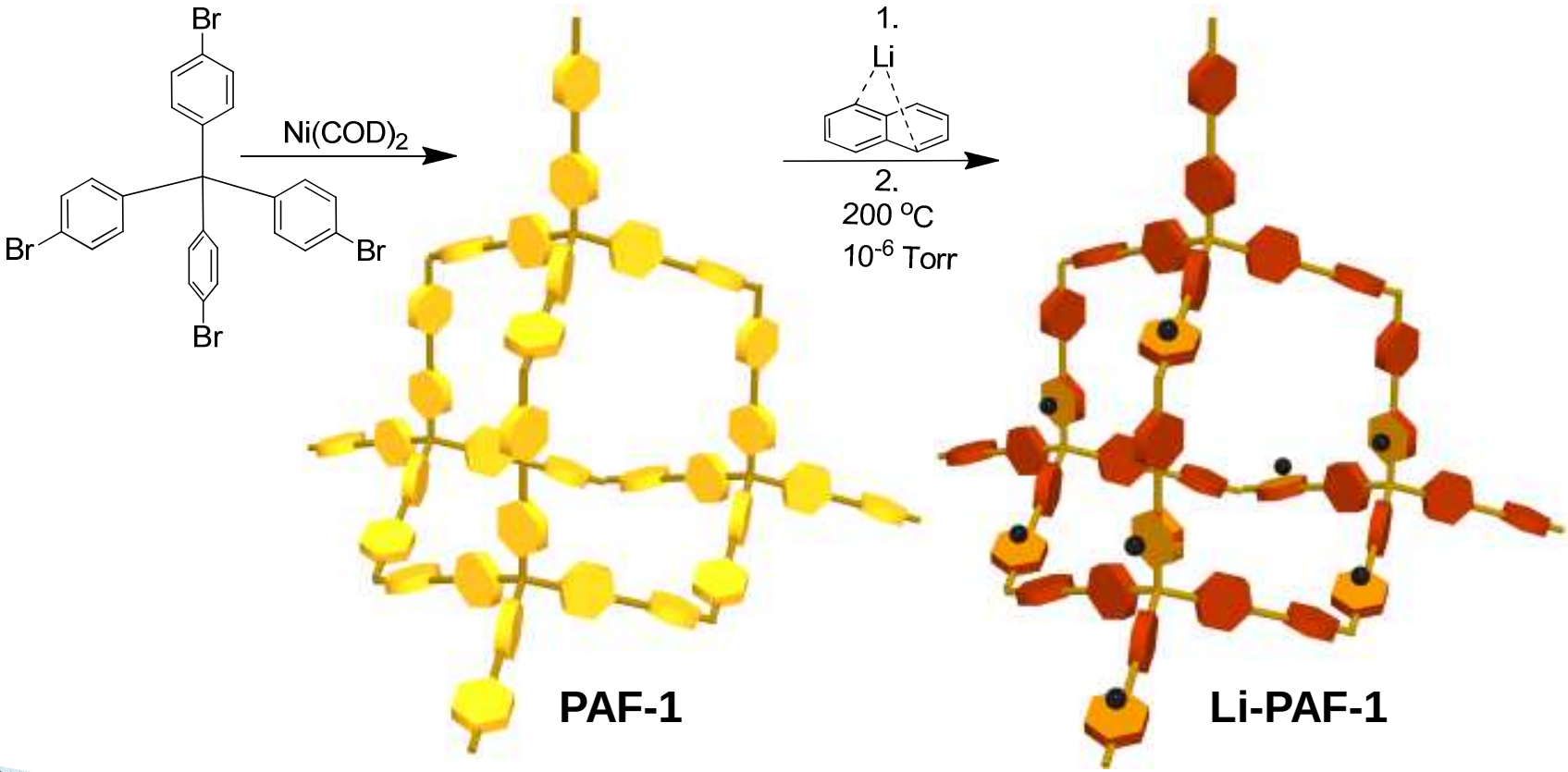


- Similar to salt or sugar crystals.
- Crystalline particles between ~20 nm and 2 mm.

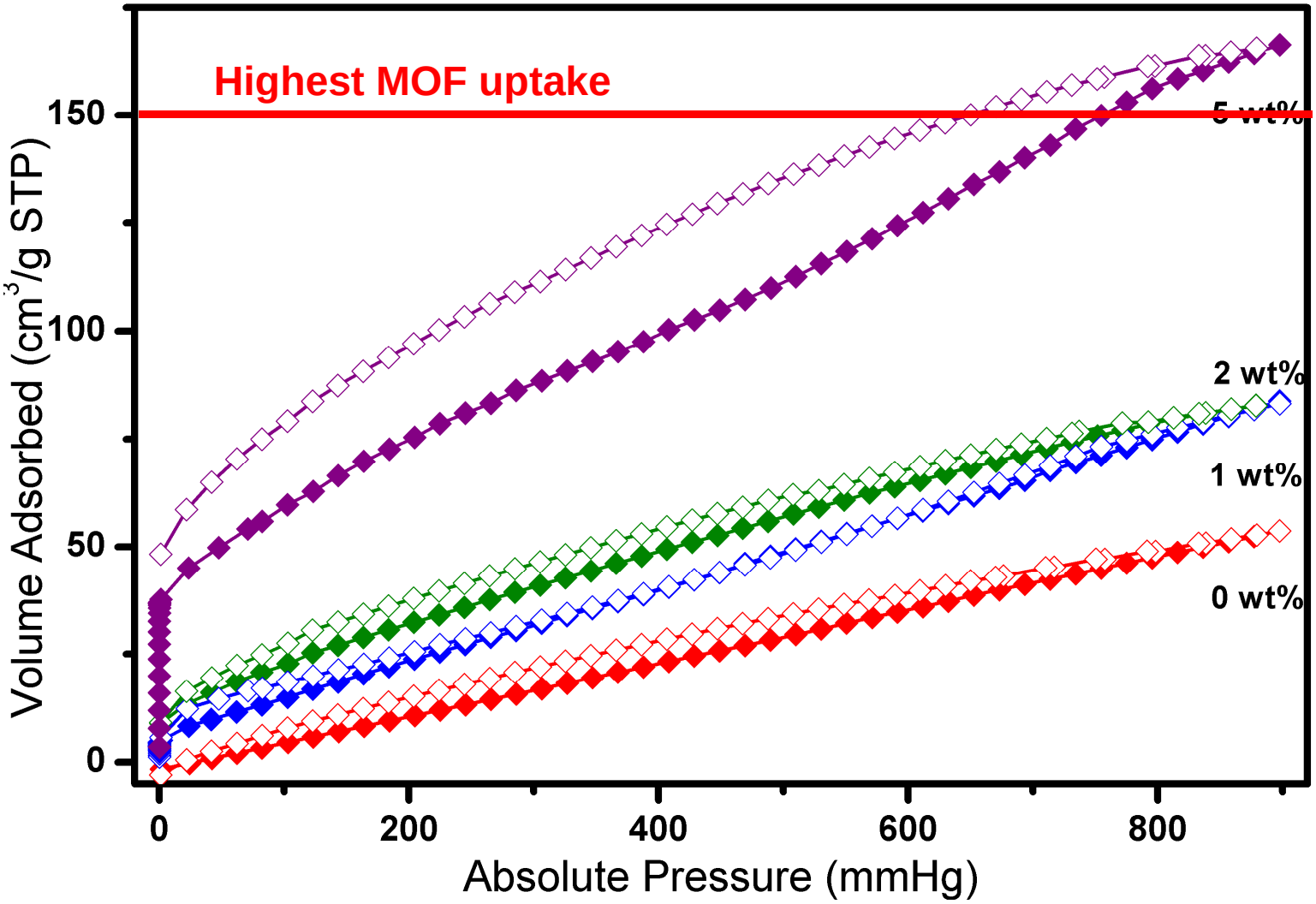
Gas Storage in MOFs



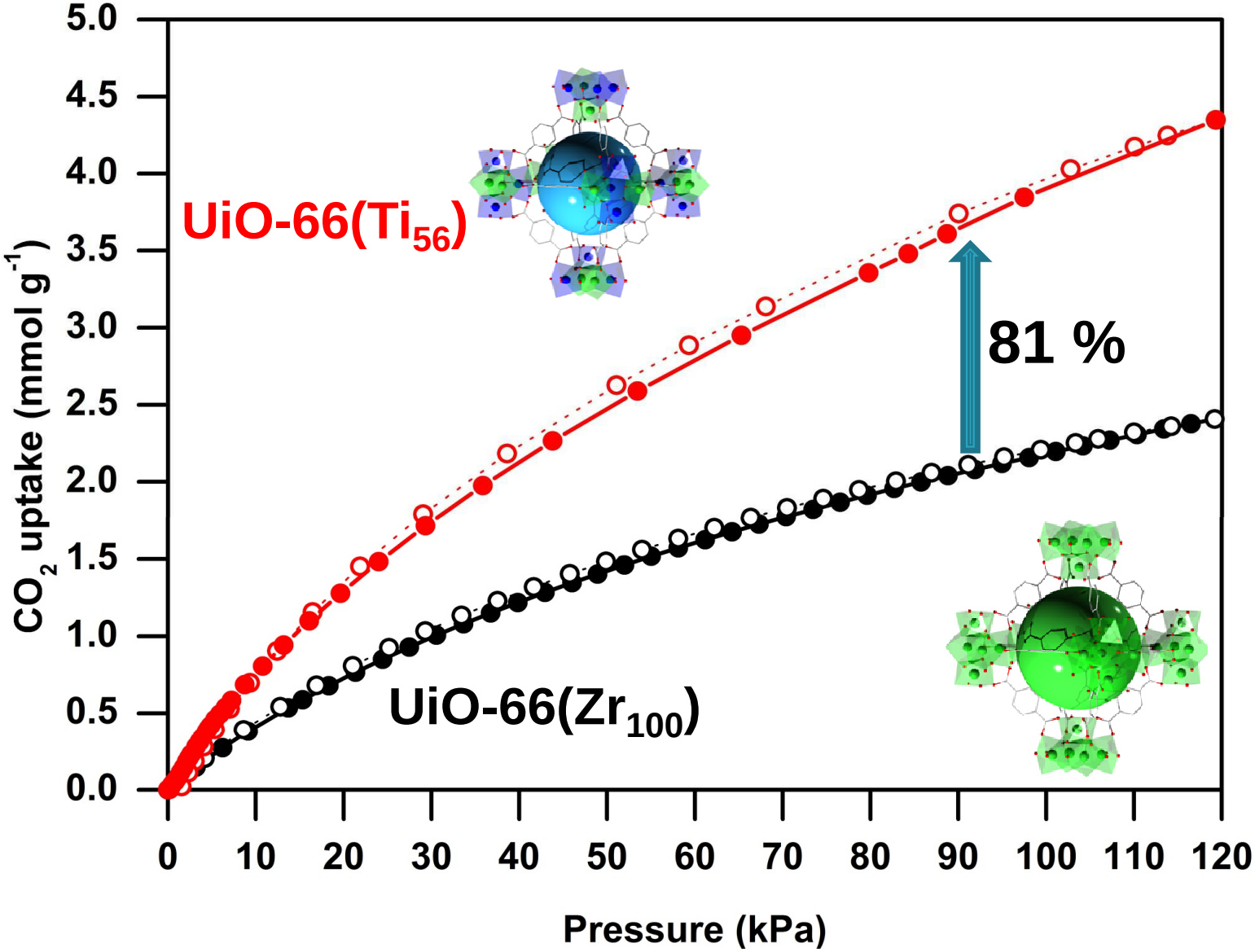
Lithiative reduction of PAFs



CO_2 uptake 273K



K. Konstas, J. W. Taylor, A. W. Thornton, W. X. Lim, B. J. Cox, J. M. Hill, T. J. Bastow, A.J. Hill, D. F. Kennedy, C. M. Doherty, C. D. Wood, M.R. Hill, *Angew. Chem. Int. Ed.*, **2012**, 51(27), 6639.

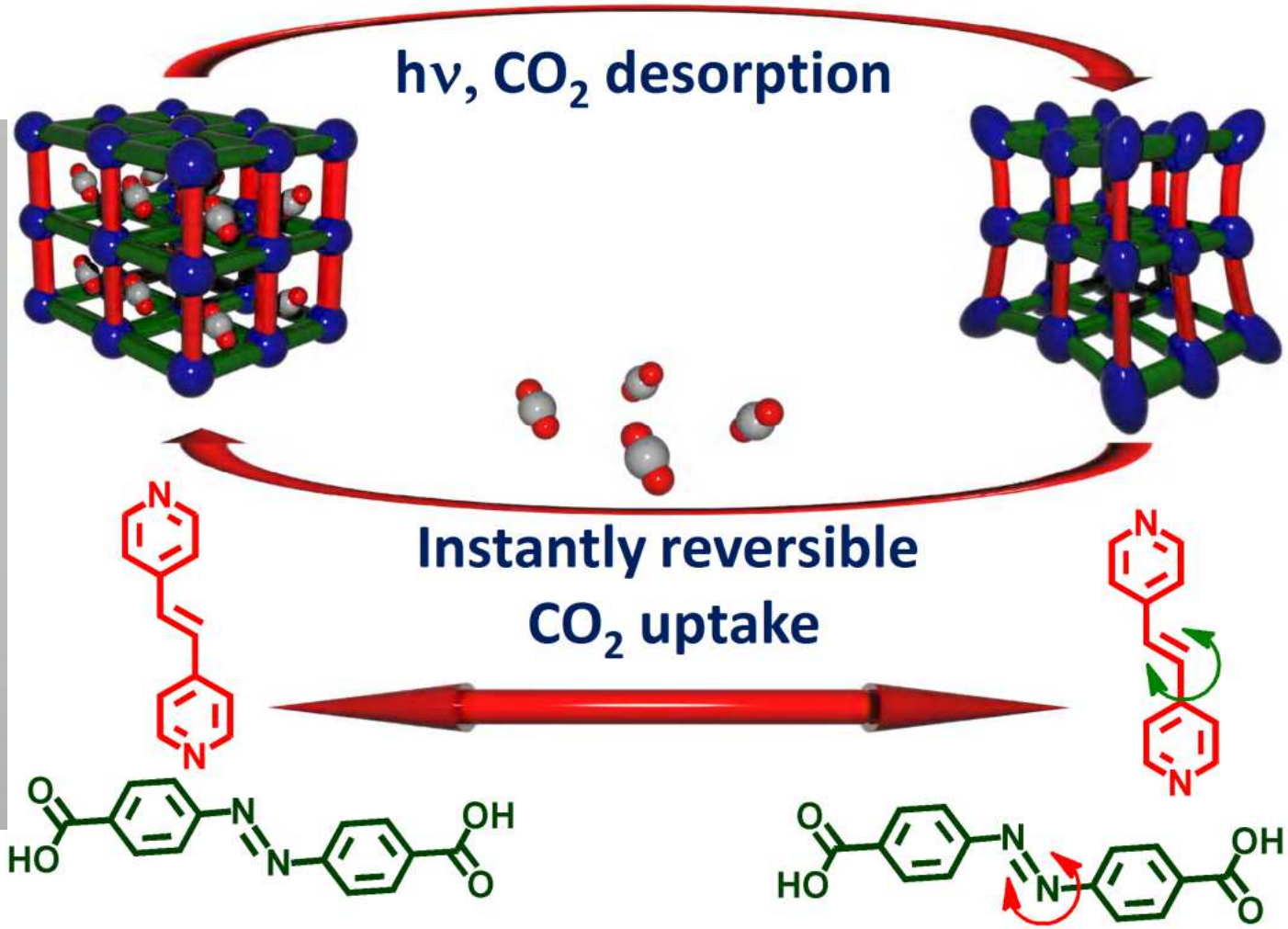


Lau, C. H.; Babarao, R.; Hill, M. R., *Chem. Commun.* **2013**, **DOI:** 10.1039/C3CC40470F, accepted with cover art.

Current CO_2 capture technology

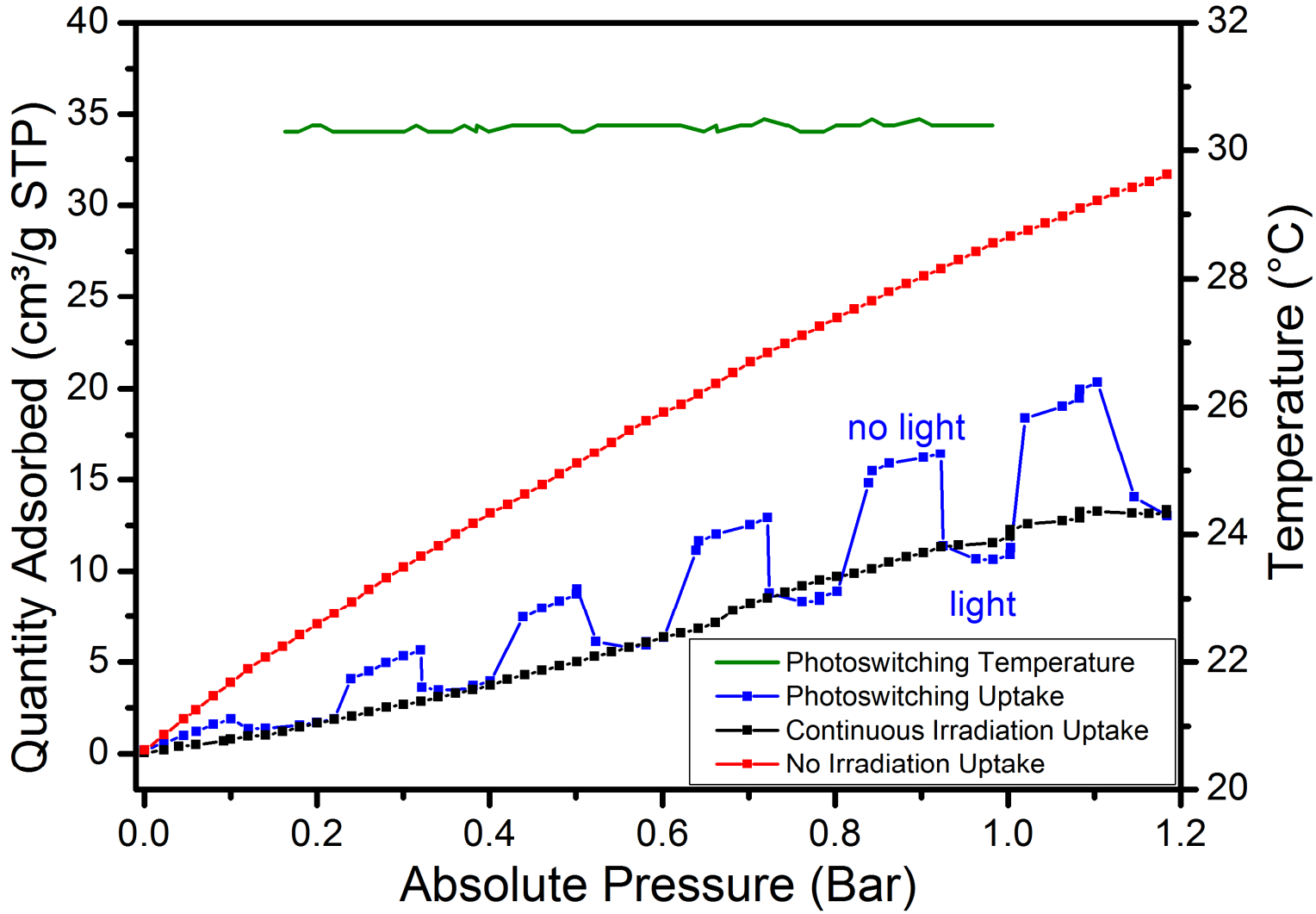
- CO_2 is captured in a 5M solution of monoethanolamine (MEA) or variants.
- This solution is heated to around to remove the CO_2, which is separated, the MEA is then re-used.
- This desorption process can use up significant fraction of the power plant's production capacity.

CO_2 release from dynamic pores

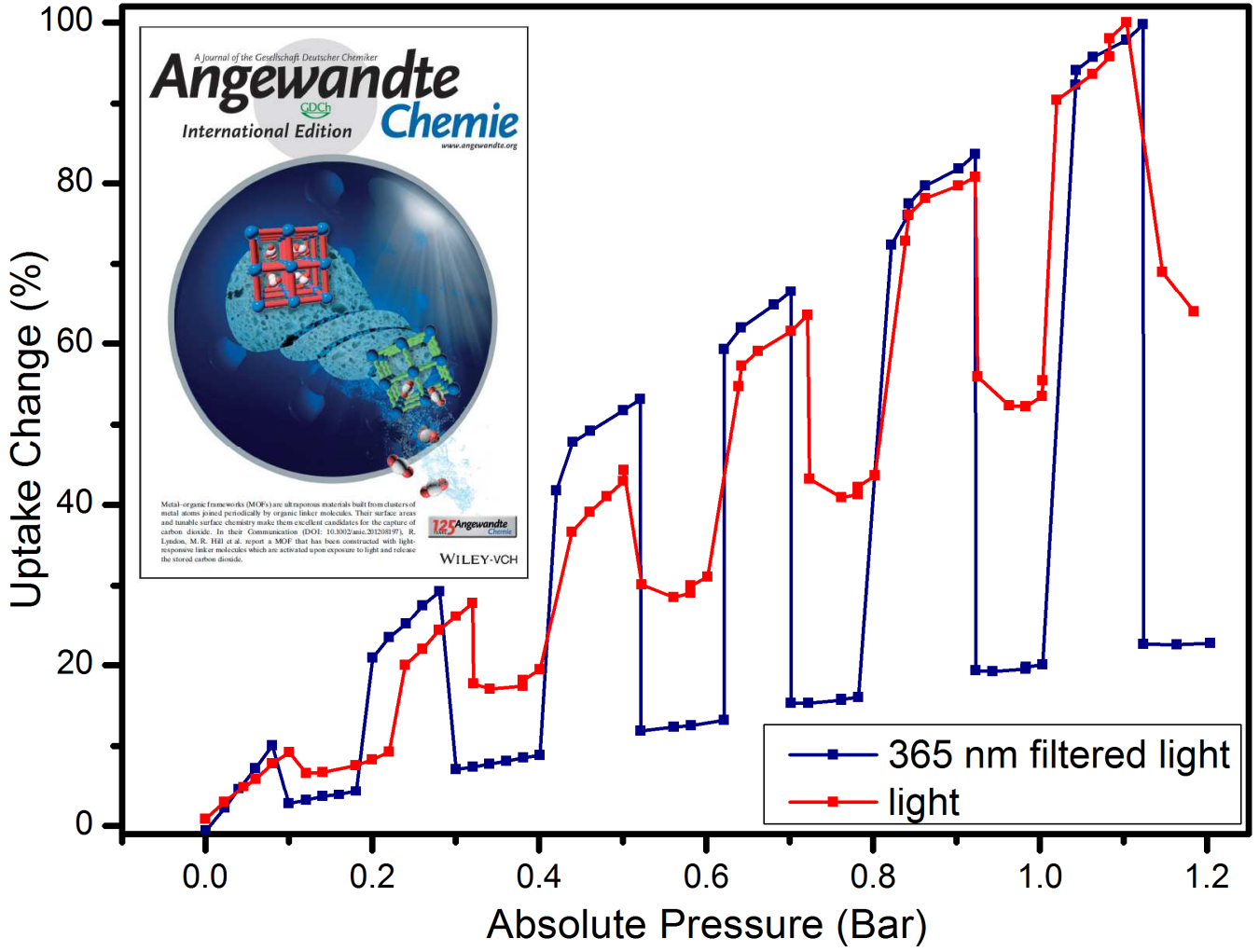


Richelle Lyndon

Light can be used to release CO_2

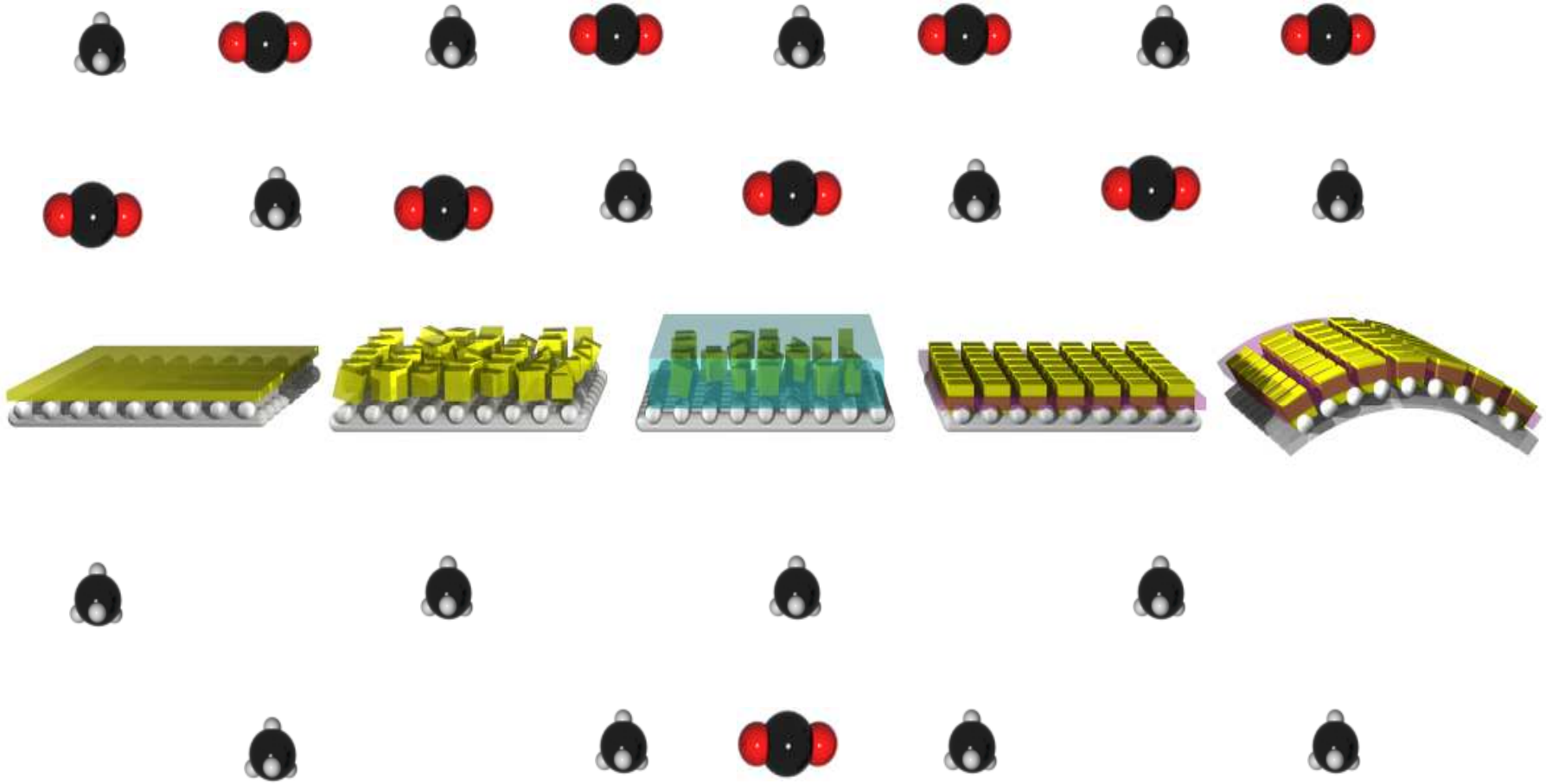


Works at optimal wavelength, or concentrated broadband UV



R. Lyndon, K. Konstas, B. P. Ladewig, P .Southon, C.J. Kepert, M.R. Hill, *Angew. Chem. Int. Ed.*, **2013**, *52* (13), 3695-3698, Lyndon, R.; Konstas, K.; Ladewig, B. P.; Hill, M. R. GAS SEPARATION PROCESSES TW8699/AU/PROV, 26-7-2012.

Gas Separations

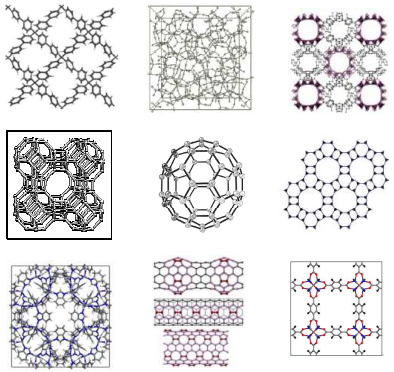


Aaron Thornton, Con Dimitrakakis, Sam Lau, Richard Noble

Virtual Hub for Screening Materials

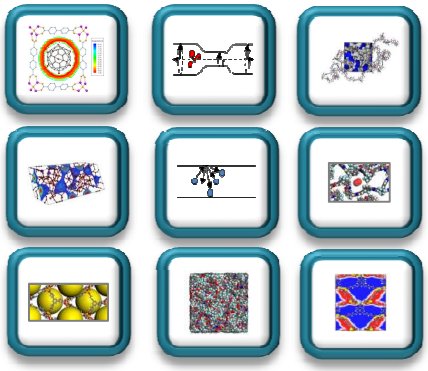
1. Candidate Materials

(> 1 Billion Structures)



2. Screening Tools

(Structure-Property Predictions)



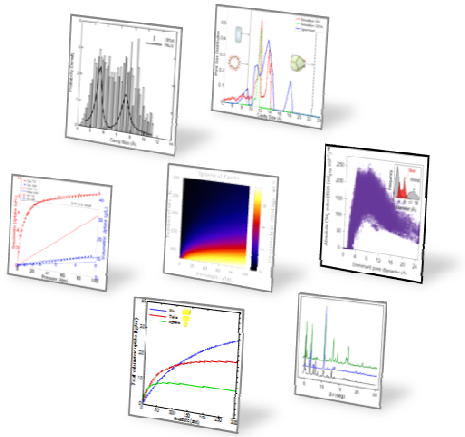
1.Adsorb IT
2.Void IT
3.Surface IT
4.Convert IT

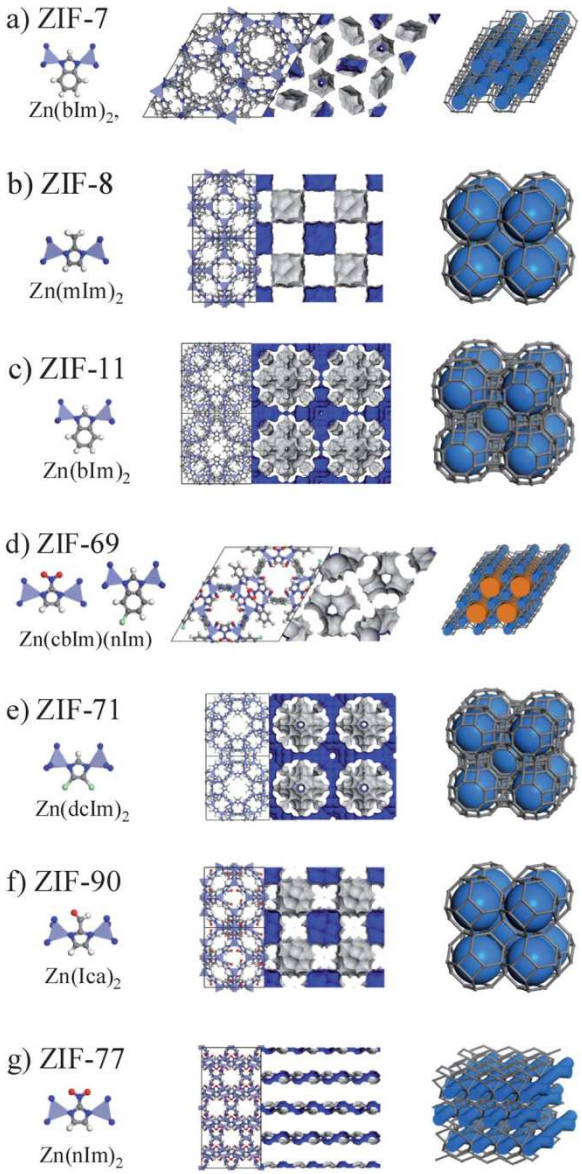
5.Pore Size IT
6.X-ray IT
7.Permeate IT
8.Simulate IT

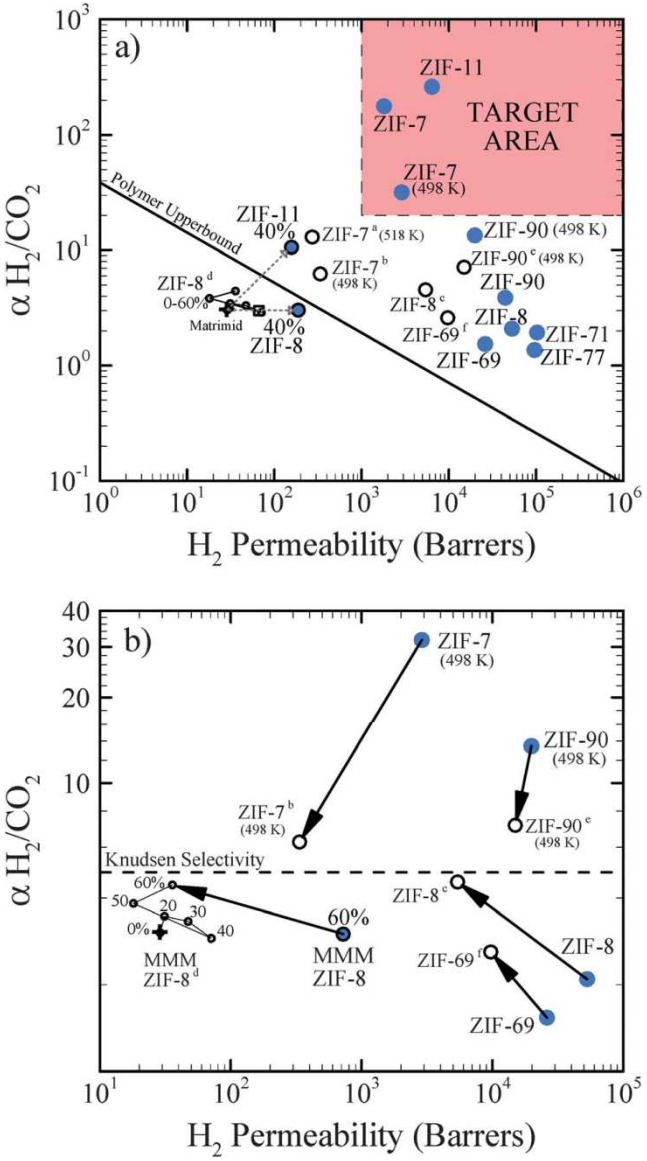
High Performance Computing

3. Promising Materials

(Meeting Industrial Feasibility Criteria)





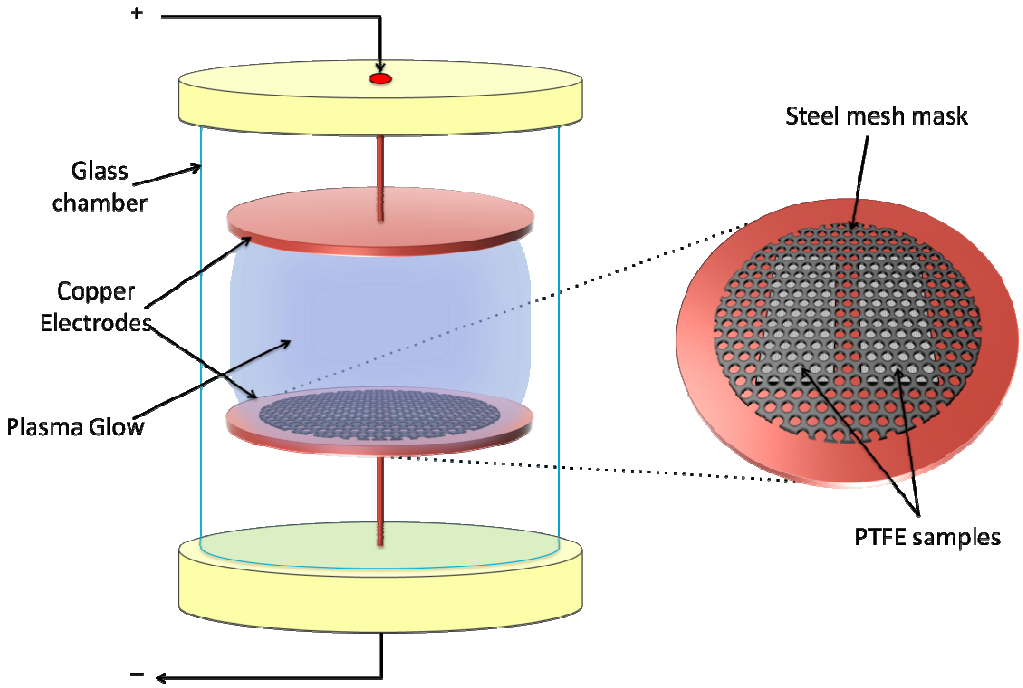


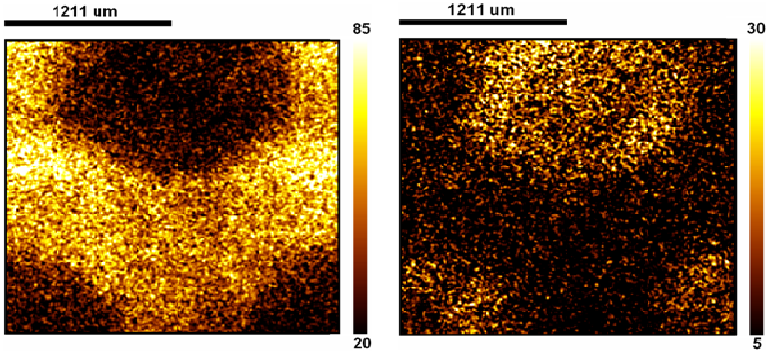
A. W. Thornton, D. Dubbeldam, M. S. Liu, B. P. Ladewig, A. Hill, M. R. Hill, *Energ. Environ. Sci.* **2012**, *5*, 7637 - 7646.

Stopping aging in glassy polymers

- Glassy polymers are attractive as gas separation membranes due to their high fractional free volume (FFV), which means there is high porosity through which gas can permeate quickly.
- Poly (1-(trimethylsilyl)-1-propyne) (PTMSP) has the highest FFV of any glassy polymer.
- However, most glassy polymers, and especially PTMSP, slowly pack into a more dense, lower FFV state, losing the fast gas permeation.
- 10 years ago this was the most active area of membrane research, but it was concluded that the aging could only be stopped by drastically lowering the permeability.

Control of ZIF growth at membrane surfaces



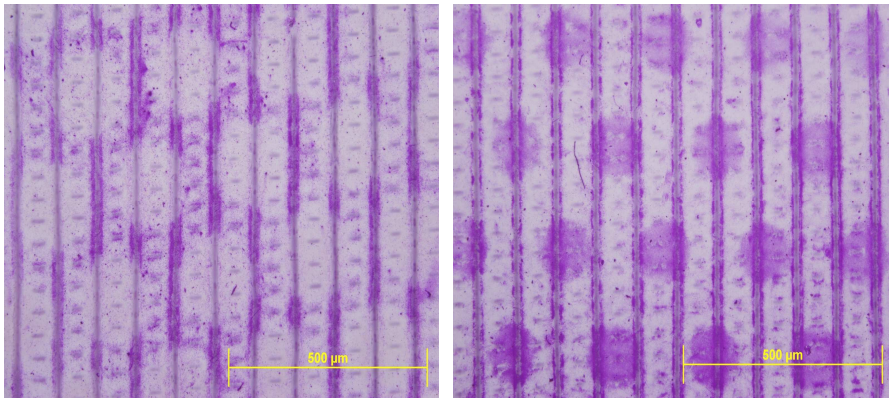


F 1s

C 1s

allylamine

diglyme



Inhibit growth

Promote growth

C. Dimitrakakis, B.W. Muir, C Easton, B.P. Ladewig, M.R. Hill, Adv Mater, **2013**, in press.

Scale up synthesis of MOFs

- Key capability challenge for any new MOF technology
- CSIRO are world leaders in scale up synthesis focussing on low energy, high speed, high sustainability processes for a range of materials.
- We have proof-of-concept that these methods work in the production of MOFs at scale.

Key CSIRO MOF capabilities

- Virtual screening for new and existing structures with potential for adsorption or separations.
- High throughput synthesis and characterisation to speed new materials discovery.
- Ability to develop large scale synthesis routes.
- Track record of working with industry partners in the MOF field.
- Platform technology IP, with 8 patents and 3 invention notes.

Thank you

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Email: matthew.hill@csiro.au
http://www.csiro.au/matthewhill