

High-throughput Computational Screening for MOF Materials Discovery: Finding a Needle in a Haystack



The
University
Of
Sheffield.

Peyman Z. Moghadam

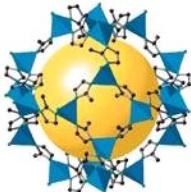
Department of Chemical and Biological Engineering
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Cambridge Crystallographic Data Centre (CCDC)

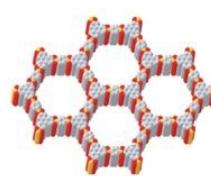
14 October 2021

My Lab Overview: Computational Materials Design and Discovery

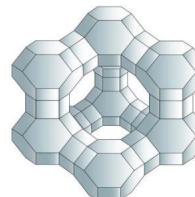
Metal-organic Frameworks



Covalent-organic Framework



Zeolites



HONDA
The Power of Dreams

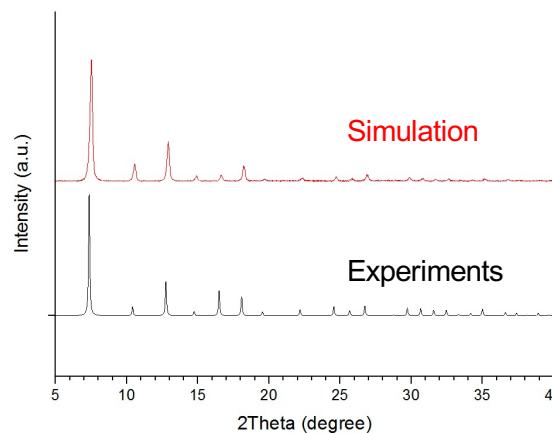
Svante

Adsorption in Porous Materials



Industrial Applications

immaterial

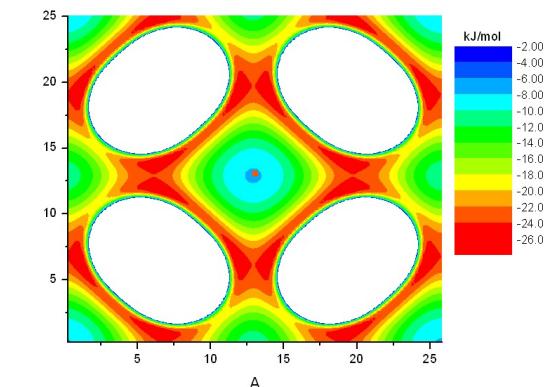
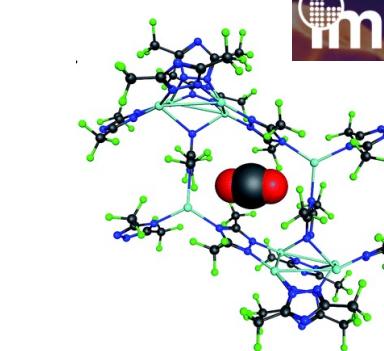
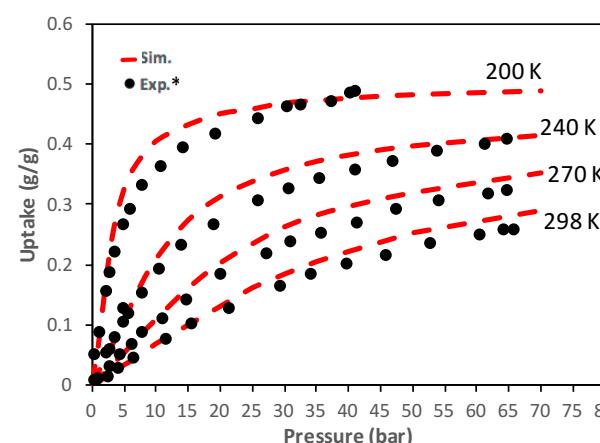


Computational Modelling

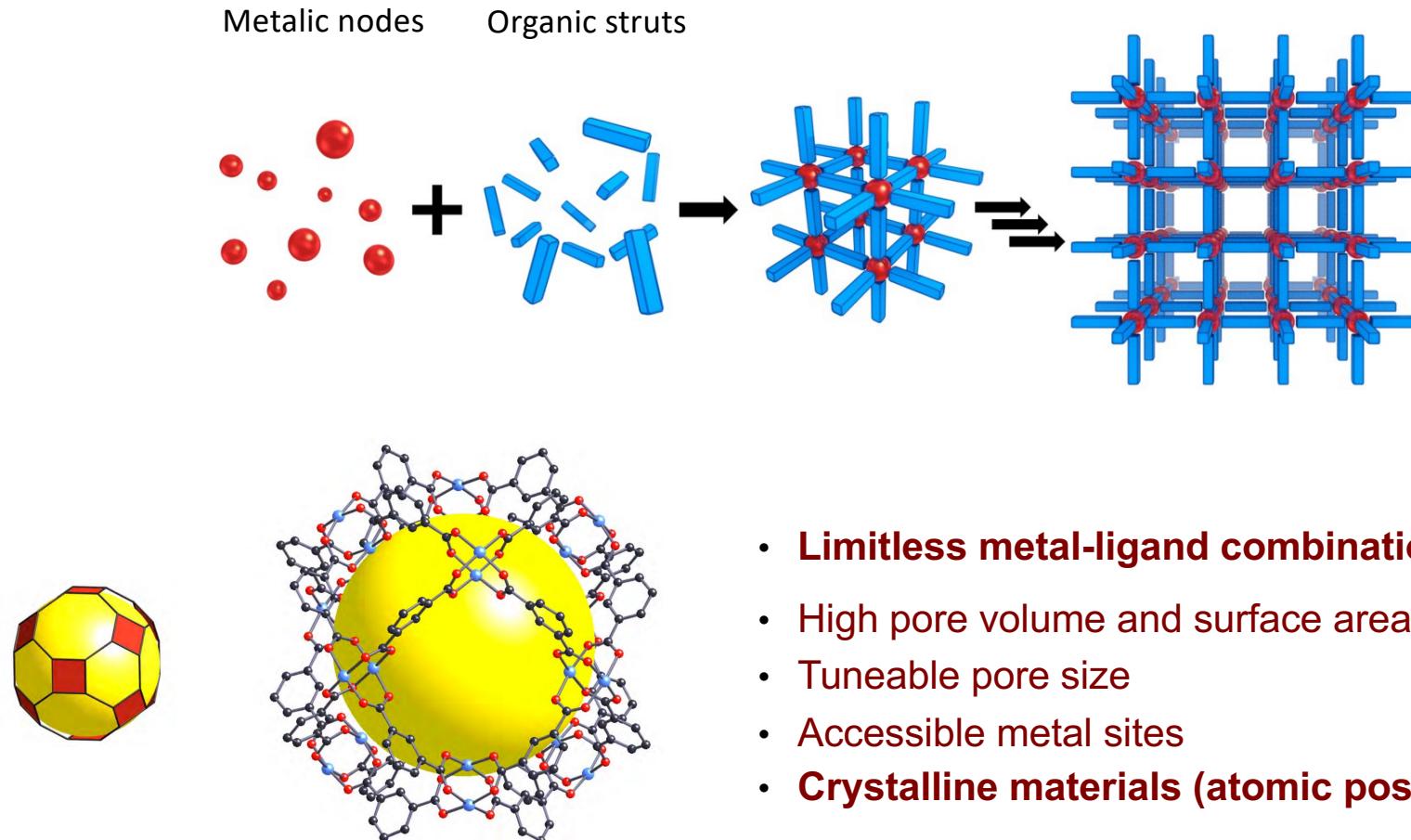
• Monte Carlo

• Quantum calculations

• Molecular Dynamics



Metal-organic Frameworks (MOFs)



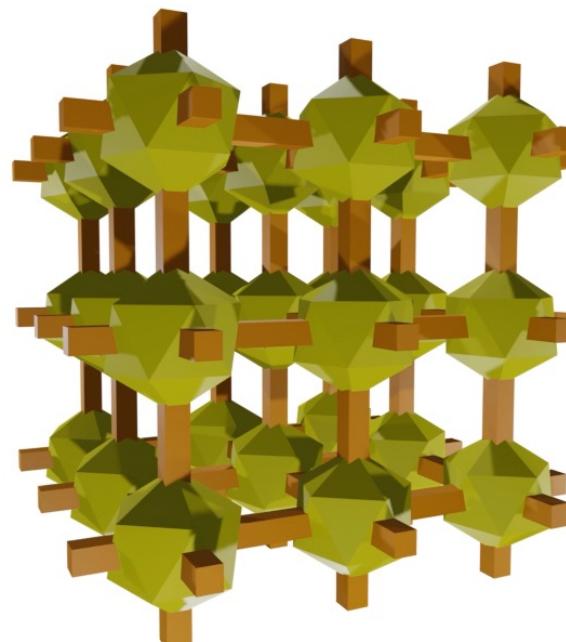
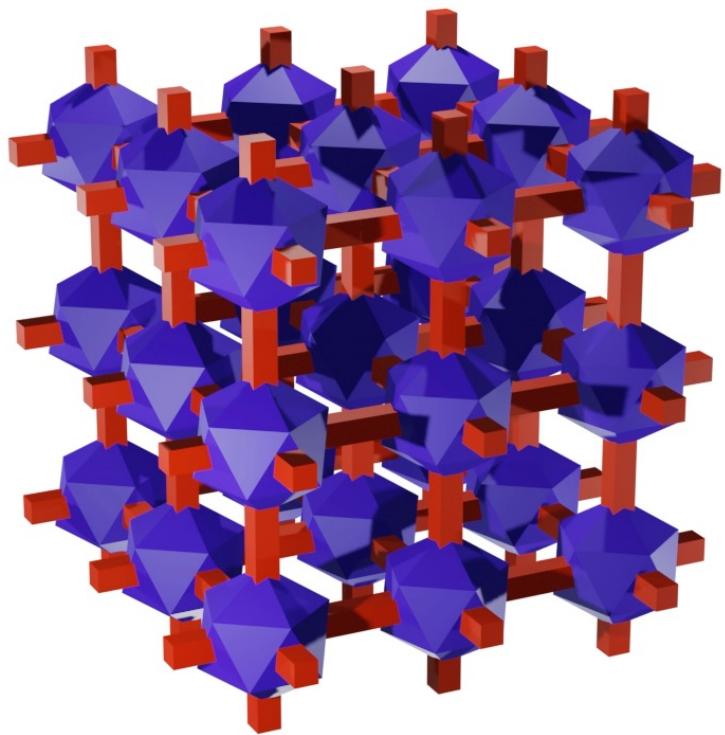
- **Limitless metal-ligand combinations**
- High pore volume and surface area
- Tuneable pore size
- Accessible metal sites
- **Crystalline materials (atomic positions known)**

Williams et al. *Science* 1999 (HKUST-1)

Yaghi et al. *Nature* 1999; *Science* 2002; *Nature* 2003 (MOF-5)

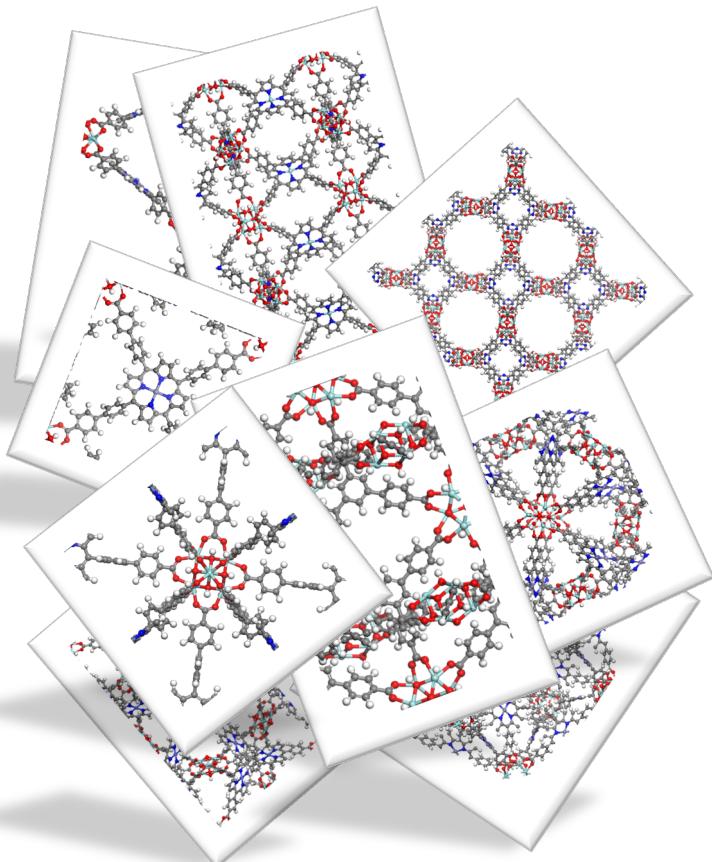
Kitagawa; Ferey; Serre; Cheetham; Kaskel; Navarro; Gascón; Long; Farha; etc.

Adsorption Phenomena Allows to Store or Separate Molecules



High-Throughput Computational Screening of MOFs

Can we **design** and **discover** MOFs on a computer prior to experiments?



Gas Storage: O_2

Gas Capture: CO_2

H_2

NH_3

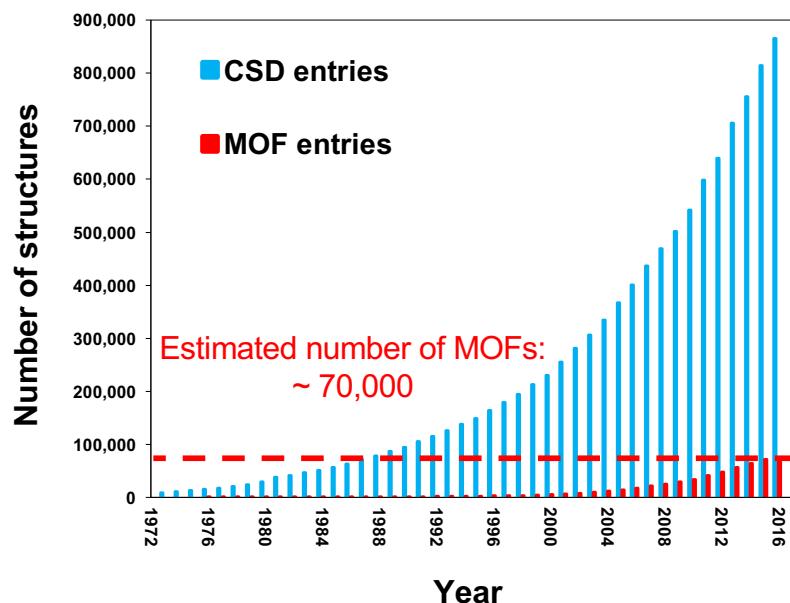
Natural gas

H_2S

VOCs

How many MOFs are out there?

The Development of the CSD MOF Subset



Using IUPAC criteria:

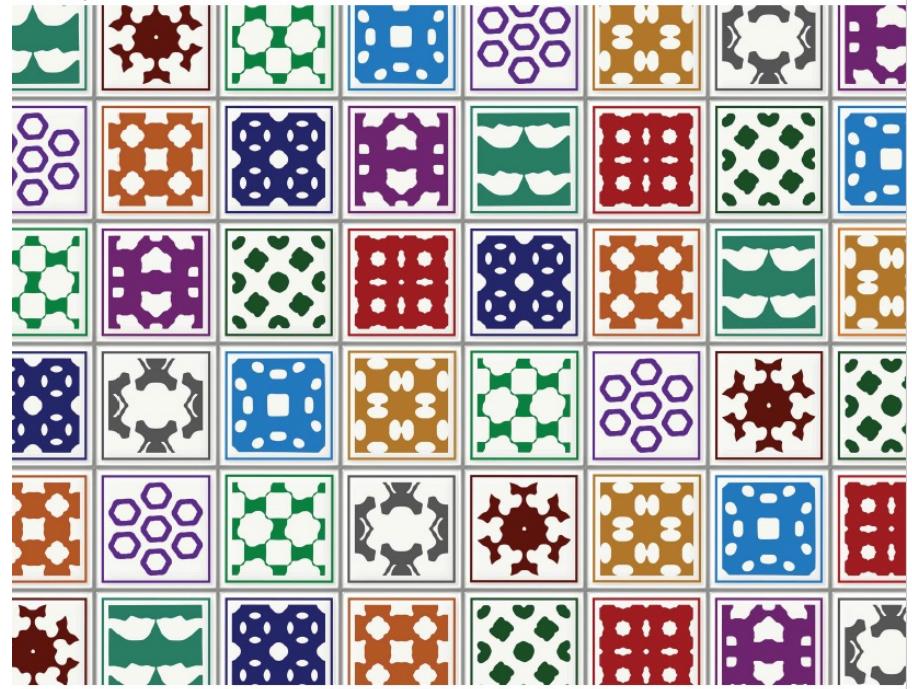
CSD MOF subset: 69,666

Non-disordered
54,808

Porous MOFs
8,388

Chemical Science

rsc.li/chemical-science



EDGE ARTICLE
Payman Z. Moghadam, David Fairen-Jimenez *et al.*
Targeted classification of metal-organic frameworks in
the Cambridge structural database (CSD)

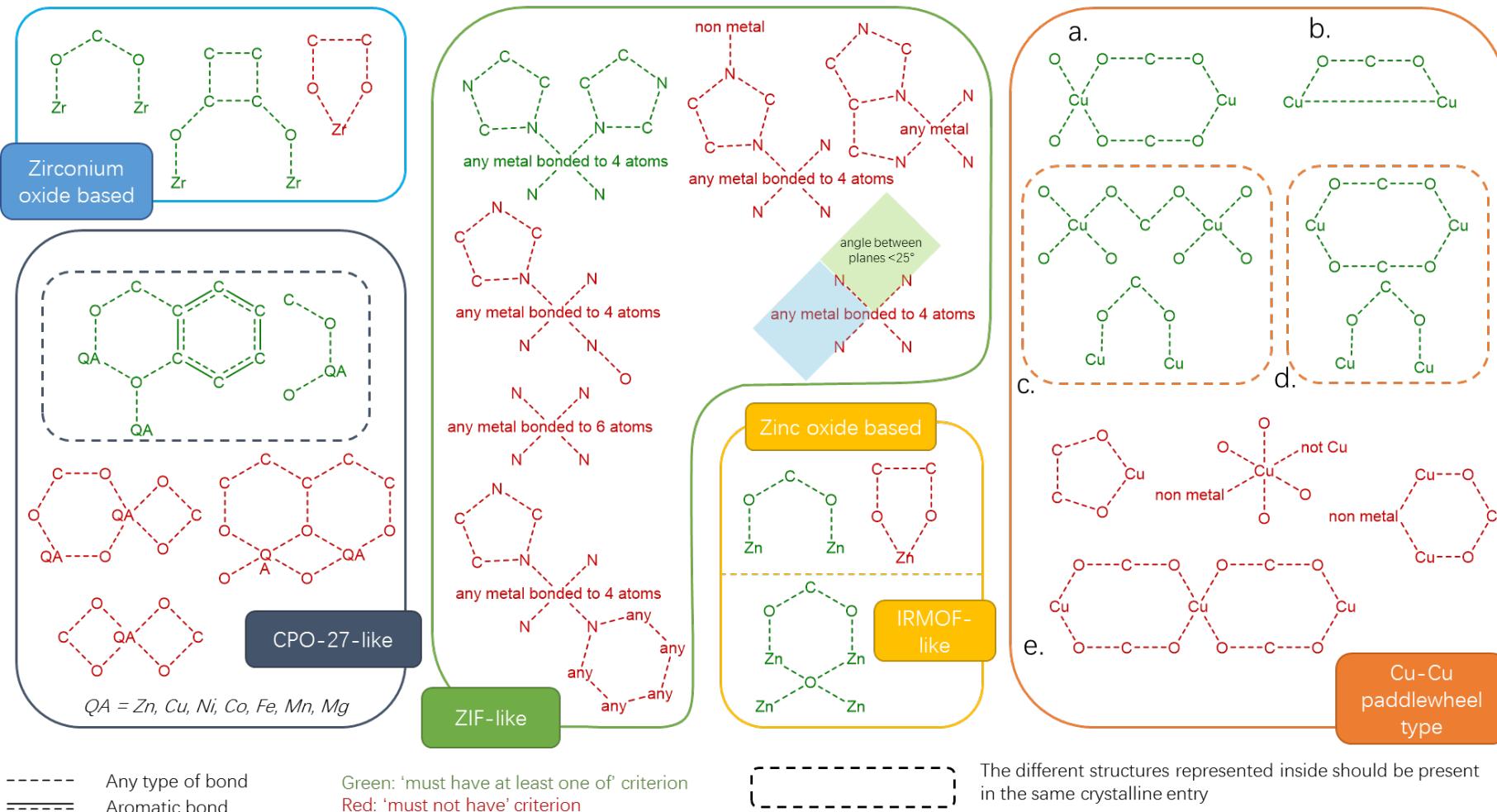


Chemistry of Materials 2017, 29, 2618
Chemical Science 2020, 11, 8373

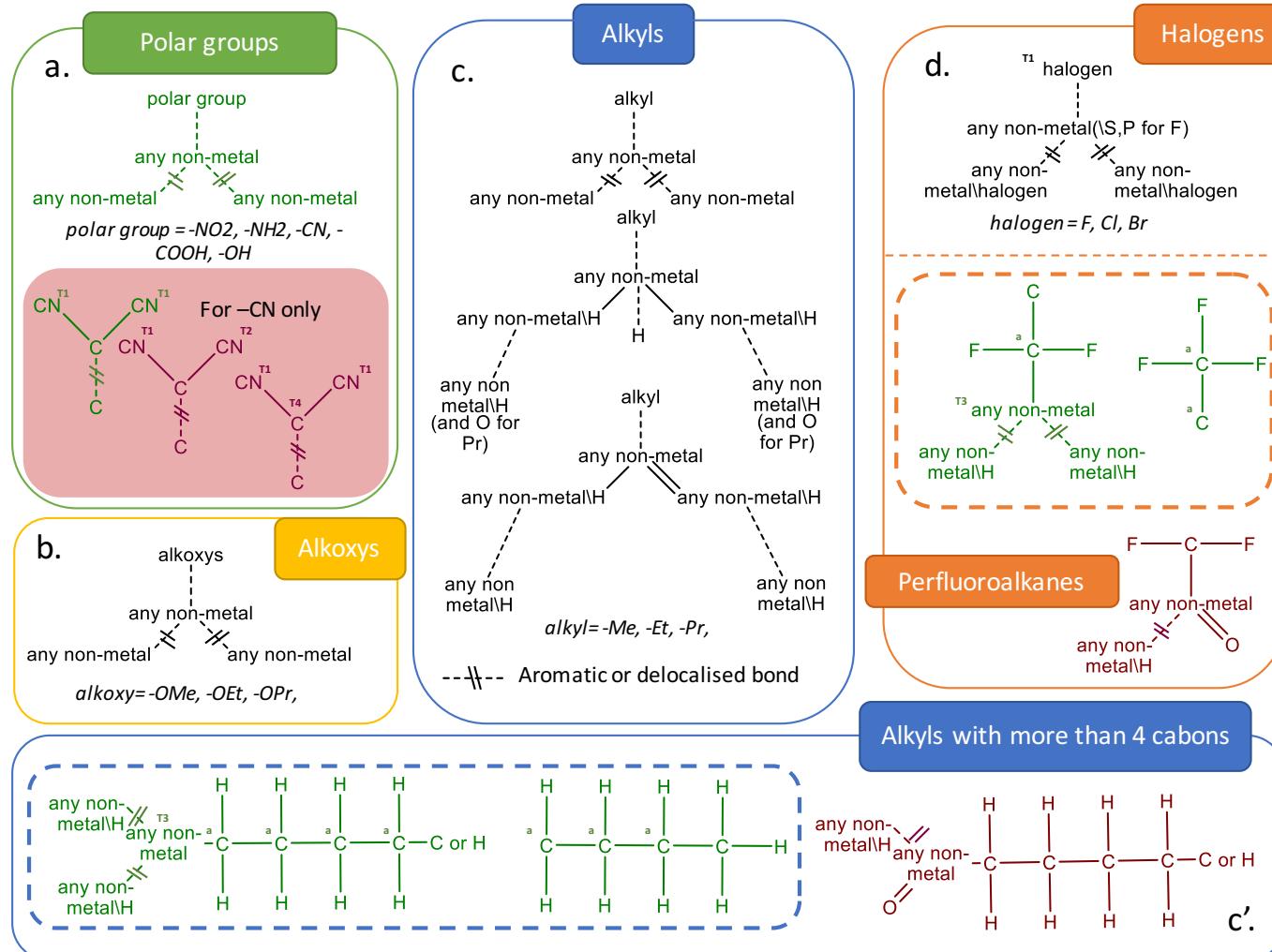


Prof. Fairen-Jimenez

Breaking Down the Big Family of MOFs into Subgroups: Inorganic Building Units



Breaking Down the Big Family of MOFs into Subgroups: Functional Groups



Eliminate structure list via hitlist combination. A ‘must not have’ in this box is a double negative.

The different structures represented inside should be present in the same entry (AND)

Green (or black when there is no combination with a ‘must not have’ criterion): ‘must have at least one of’ criterion

Red: 'must not have' criterion

— Single bond

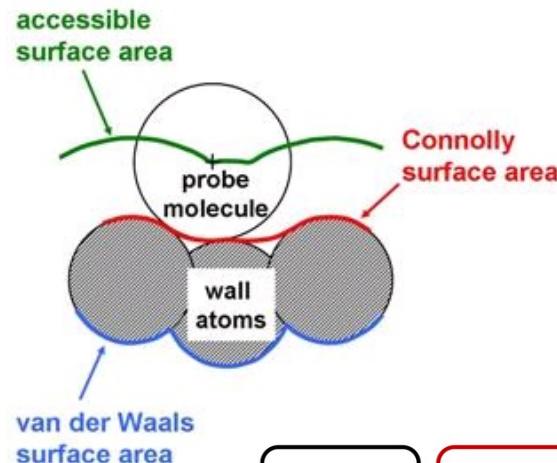
----- Any type of bond

--\!-- **Single, double, aromatic or delocalised bond, unless otherwise specified.**

Tn: The corresponding atom is bonded to n atoms

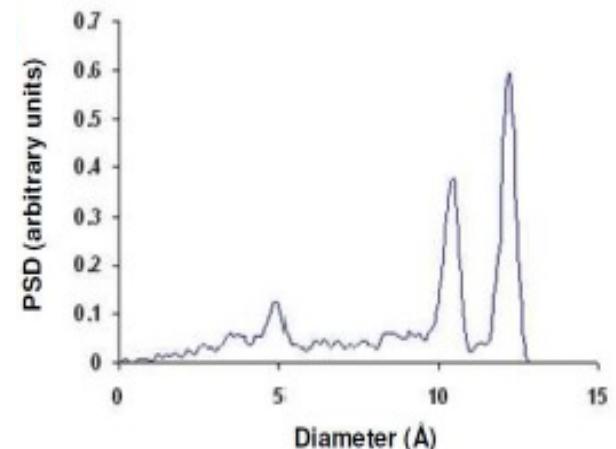
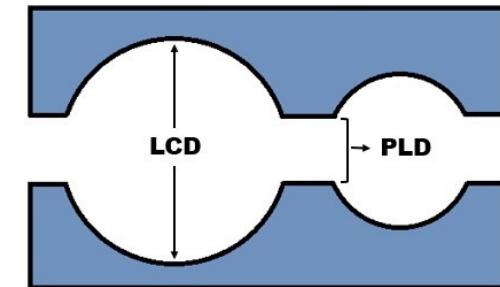
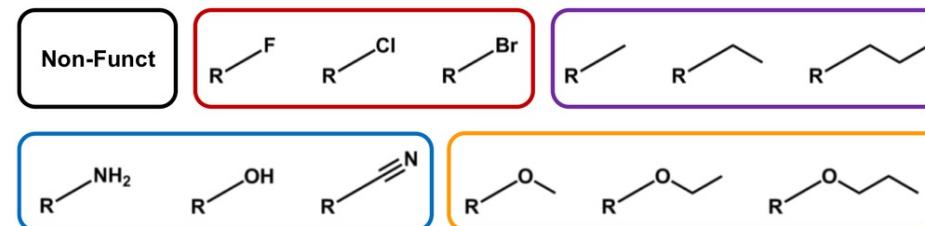
Upperscript a: the atom is acyclic

Computational characterisation of CSD MOF structures



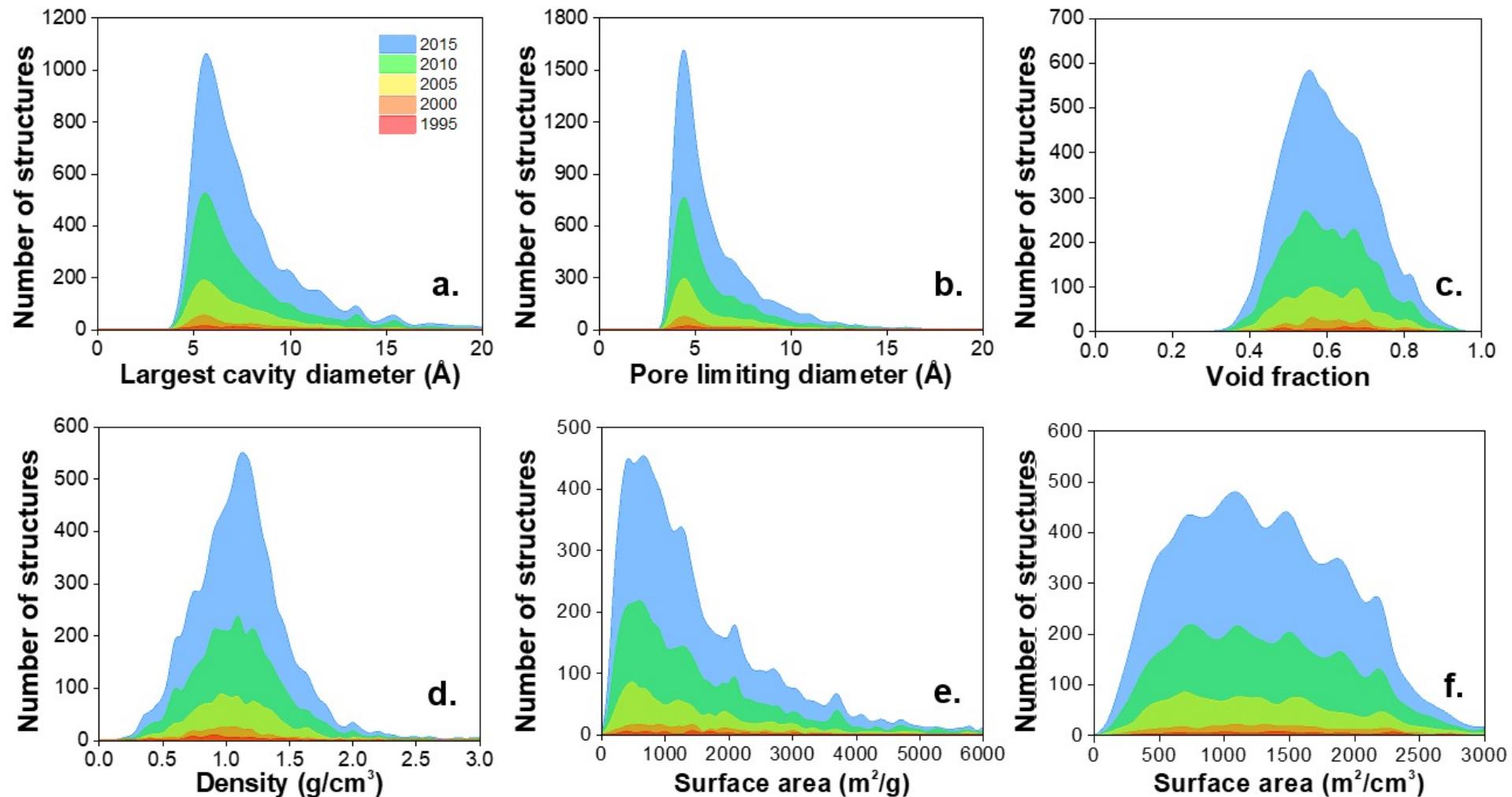
MOF properties

Pore size distribution
Accessible/BET area
Surface chemistry

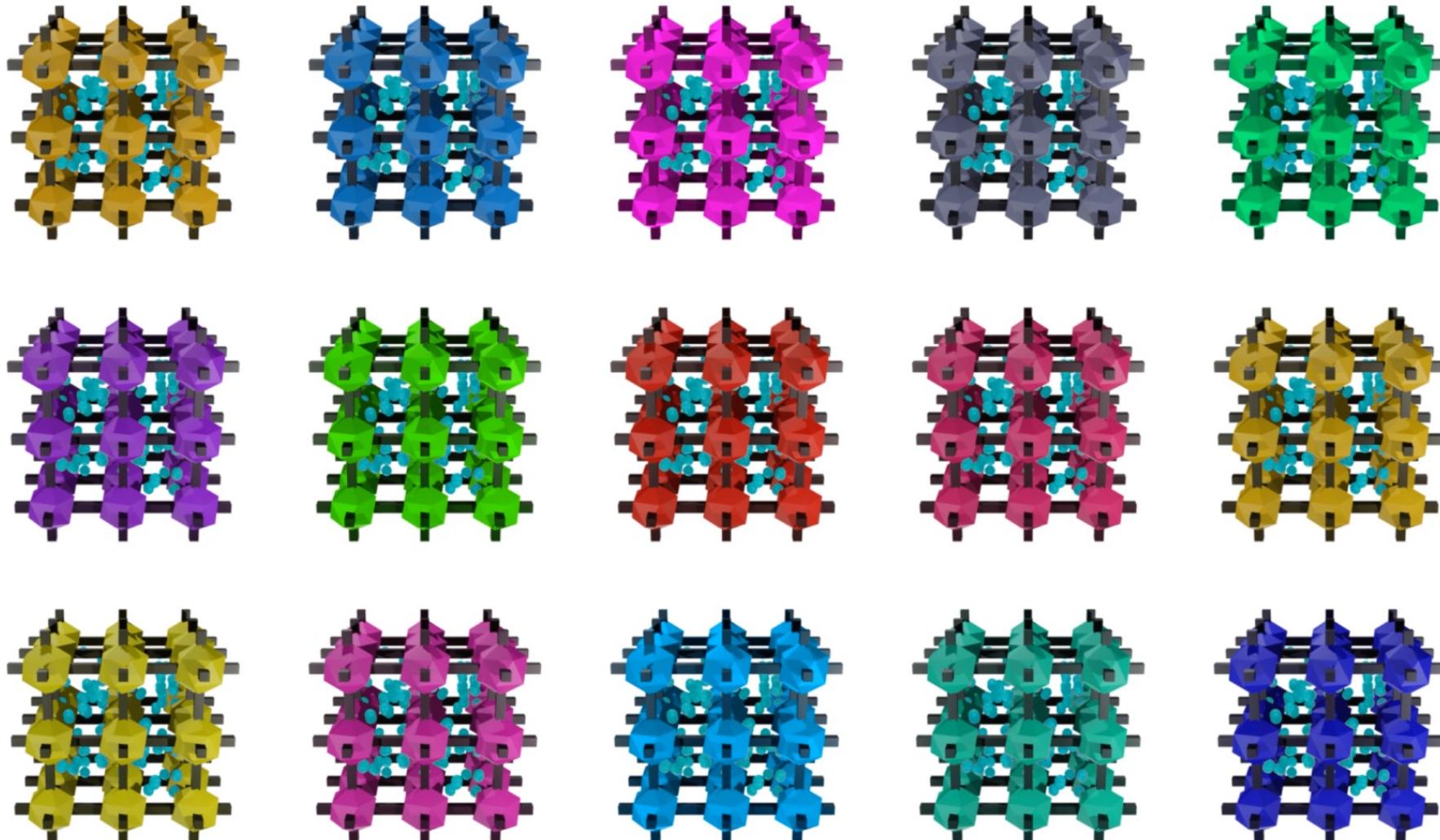


- Providing valuable information about the expected adsorption performance of the materials
- Assessing the quality of experimental samples
- Faster than experiments

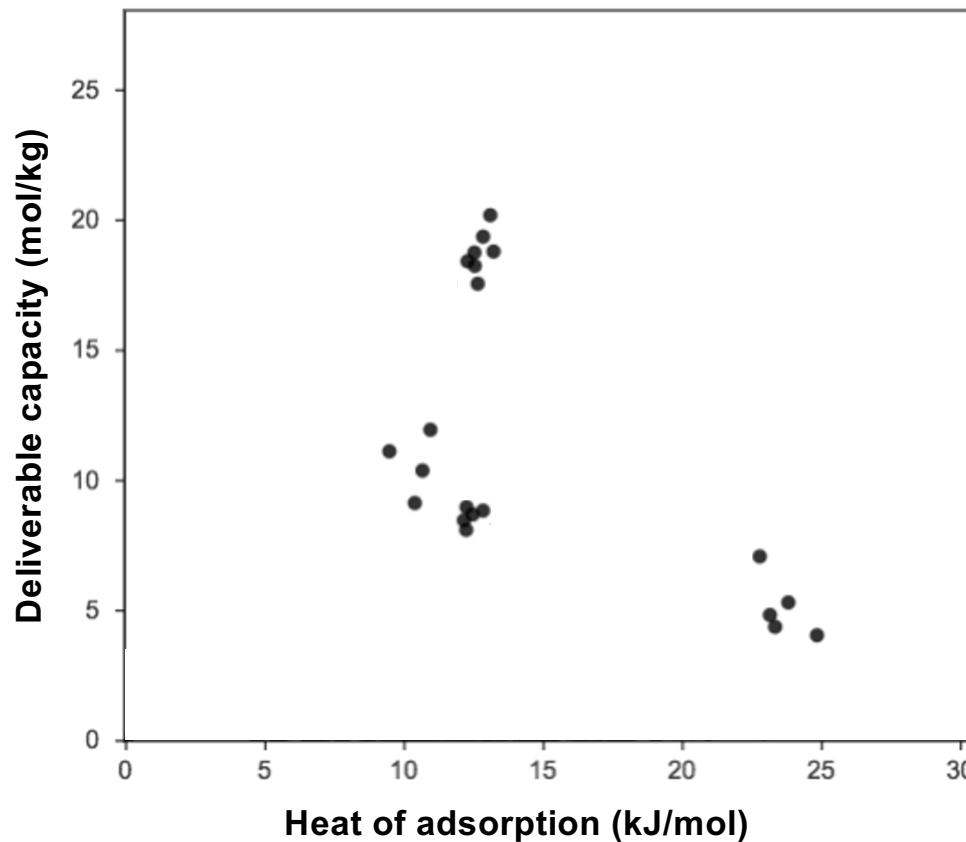
Geometric characterisation of CSD MOF structures



Monte Carlo Simulations Allows Fast High-Throughput Screening (HTS)

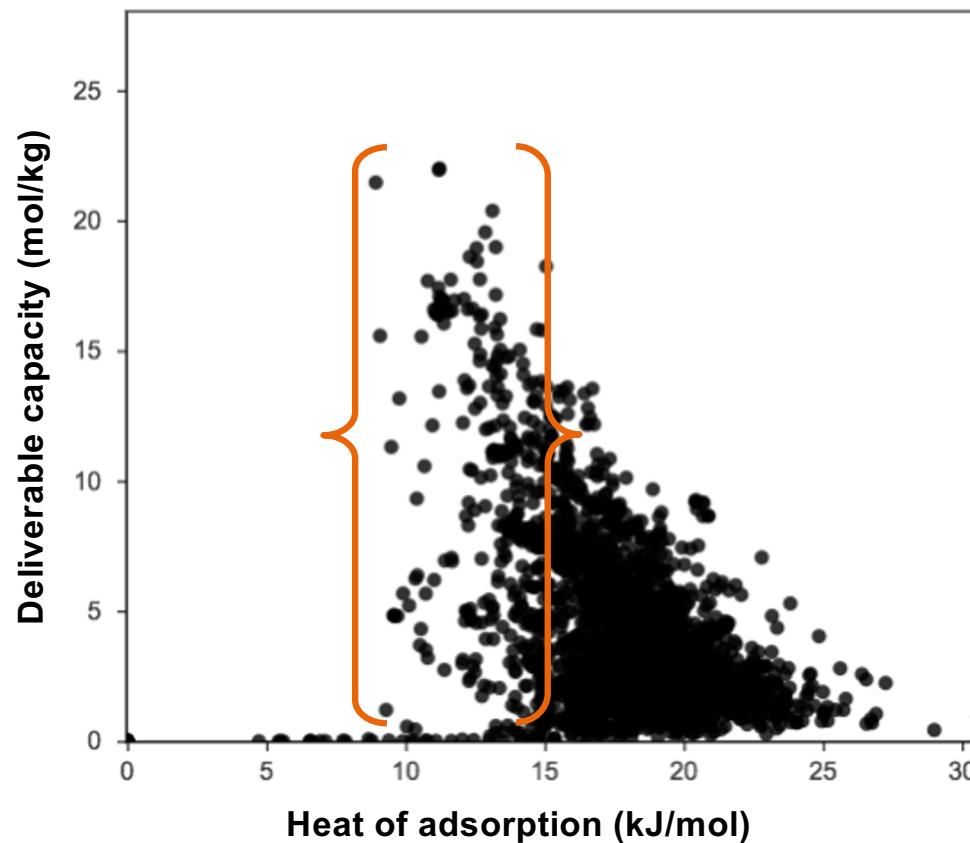


High-throughput Screening of MOFs for Oxygen Storage: From Small Data to Big Data

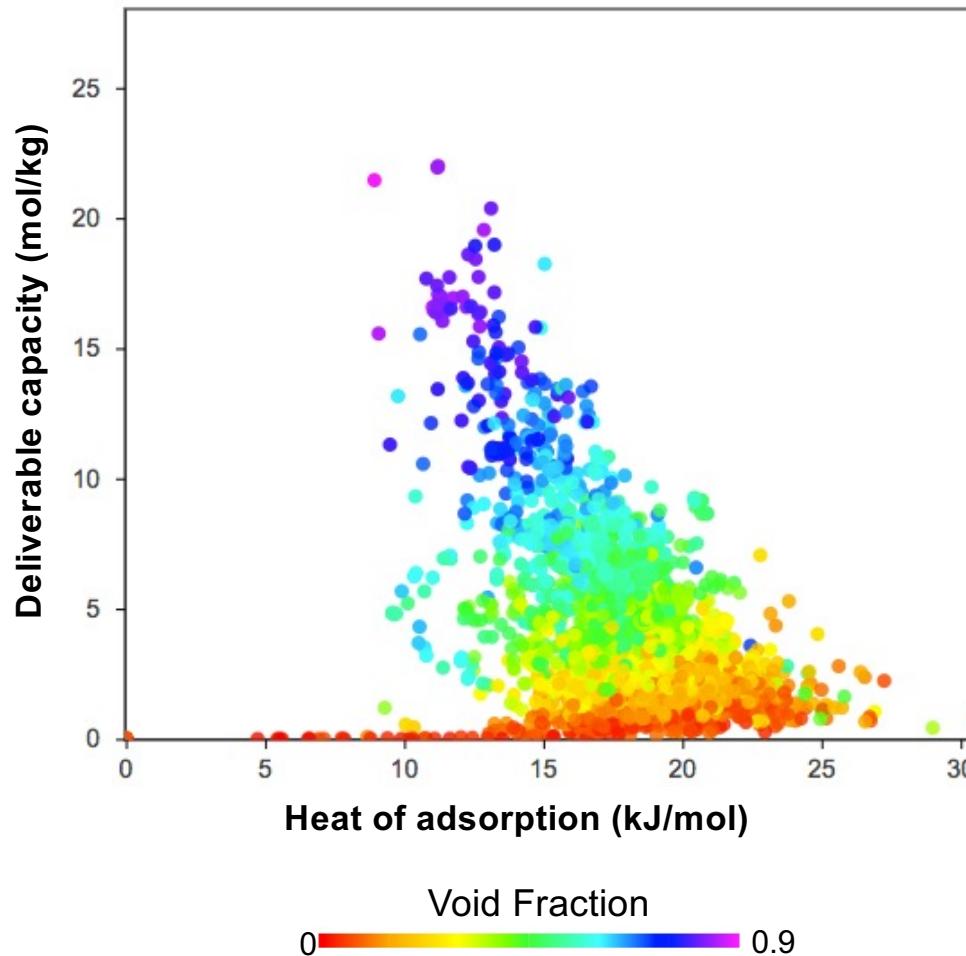


Oxygen deliverable capacity = uptake at P_{storage} (140 bar) – uptake at P_{release} (5 bar)

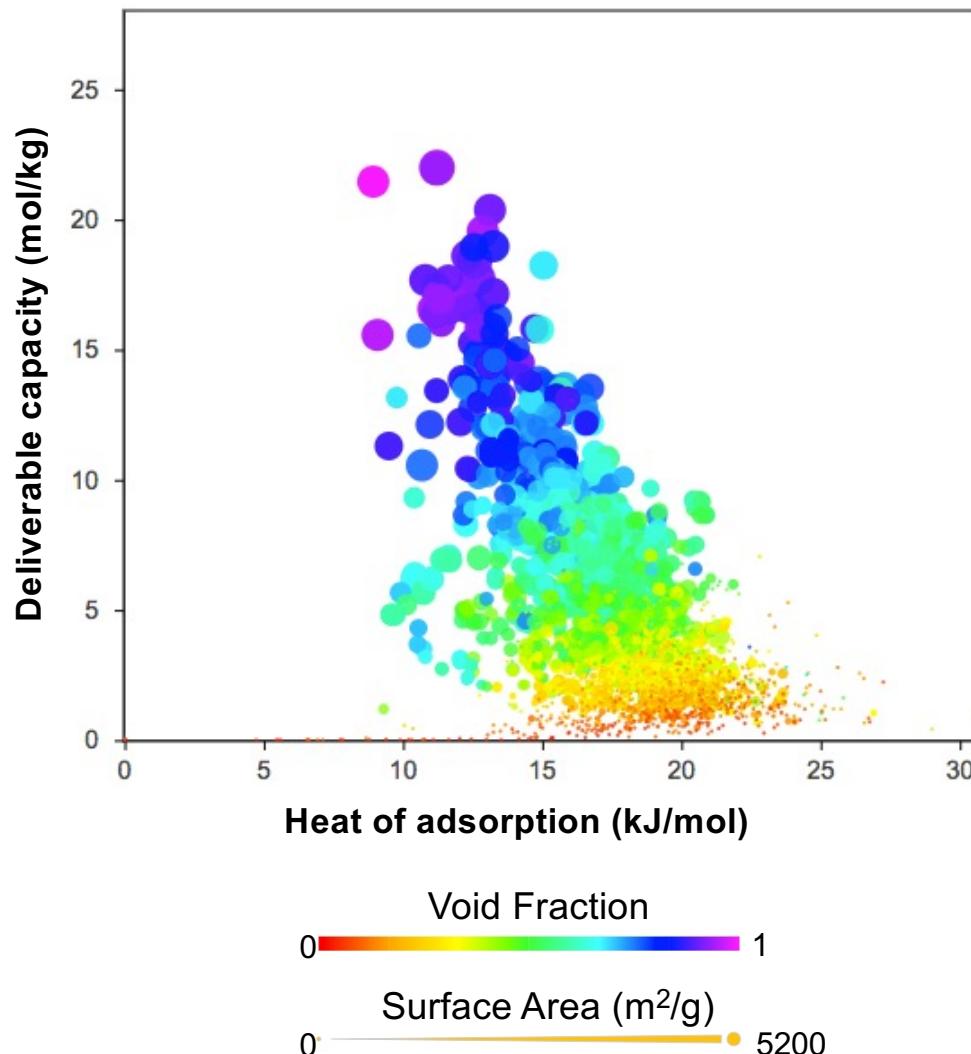
From Big Data to Knowledge: Performance-property Relationships



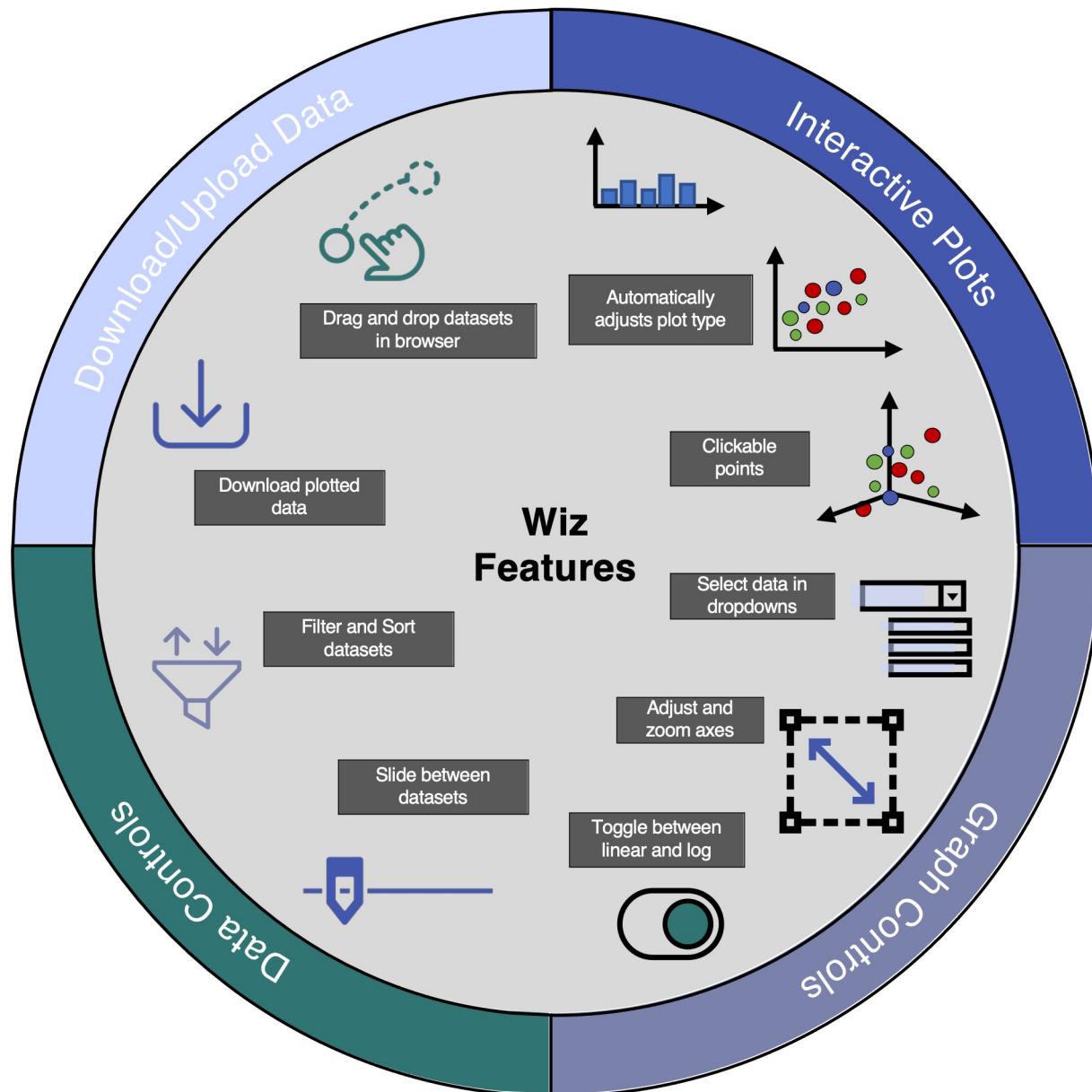
From Big Data to Knowledge: Performance-property Relationships



From Big Data to Knowledge: Performance-property Relationships



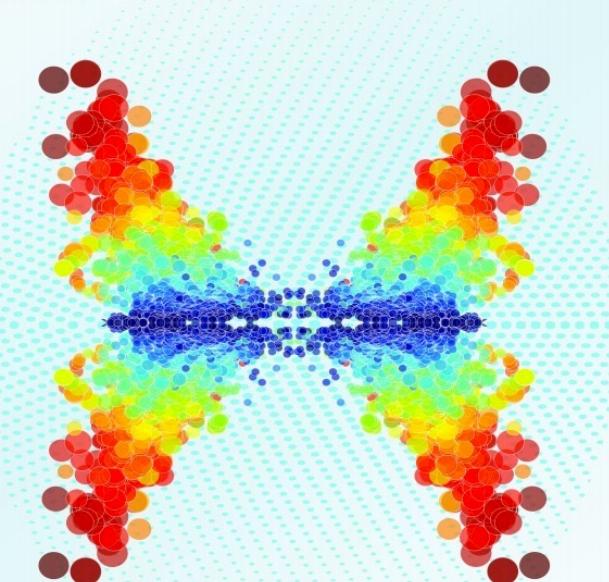
Wiz: A Web-Based Tool for Interactive Visualization of Big Data



<https://wiz.shef.ac.uk/>

Patterns

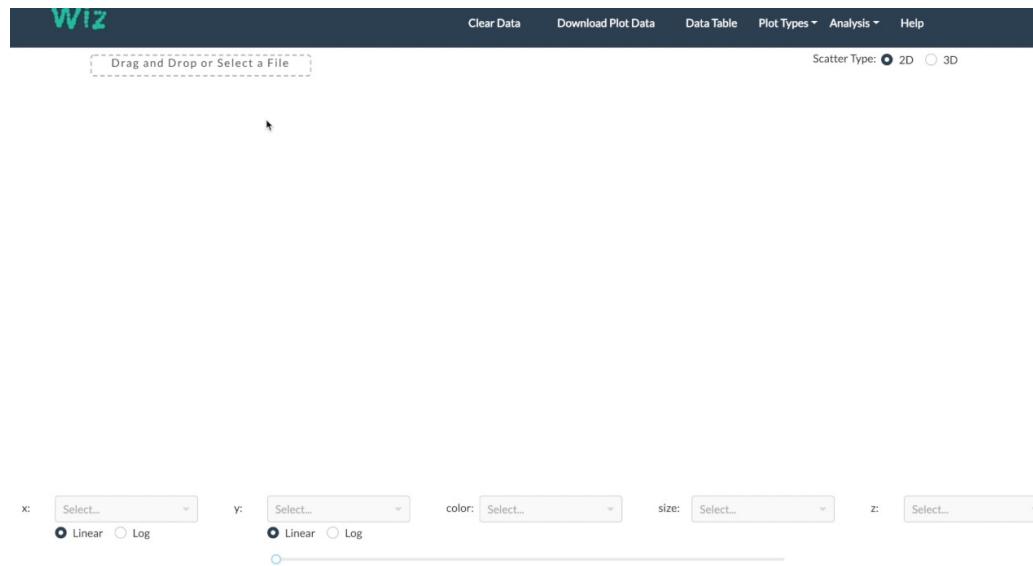
Volume 123
Number 2
August 18, 2020



CellPress

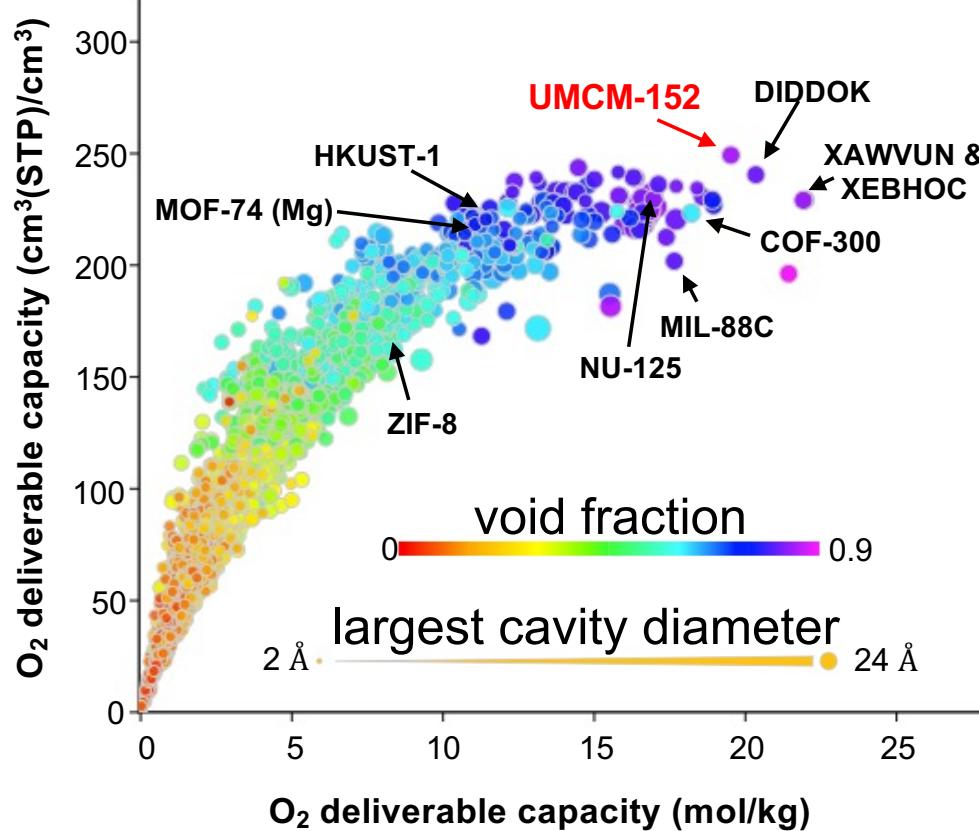
Patterns 2020, 1, 100107

Wiz for Real-time Data Analysis

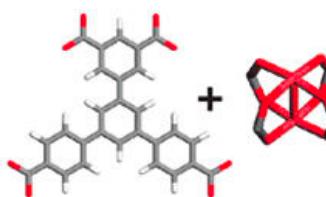
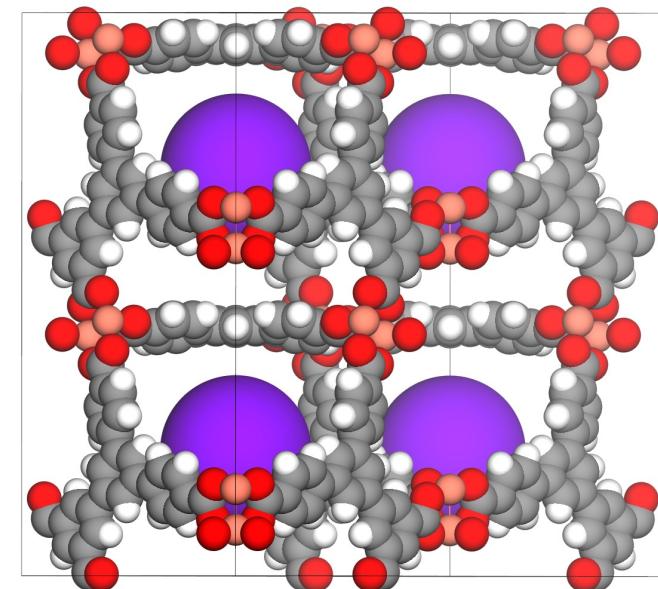


<https://wiz.shef.ac.uk/>

HTS for Oxygen Storage: Top candidates



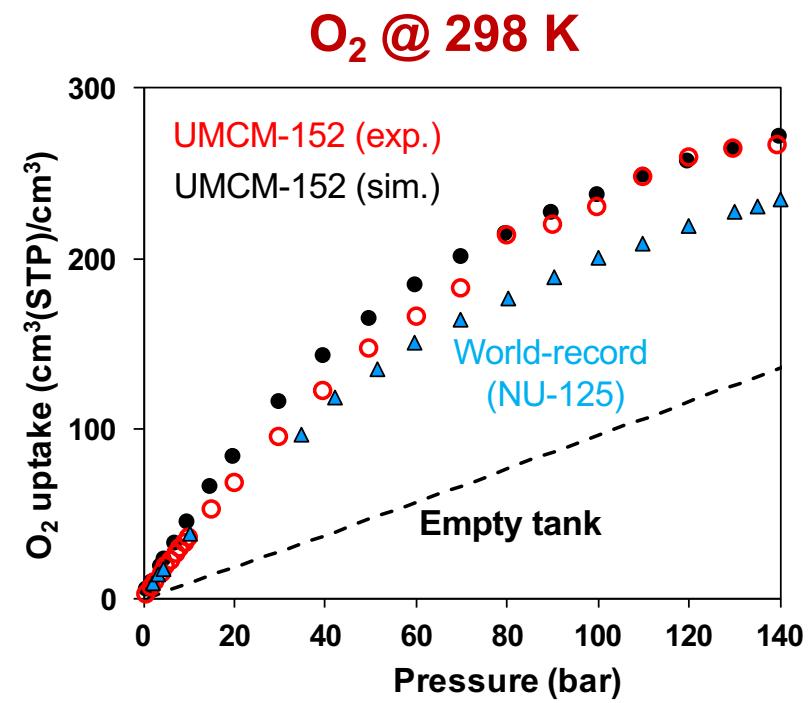
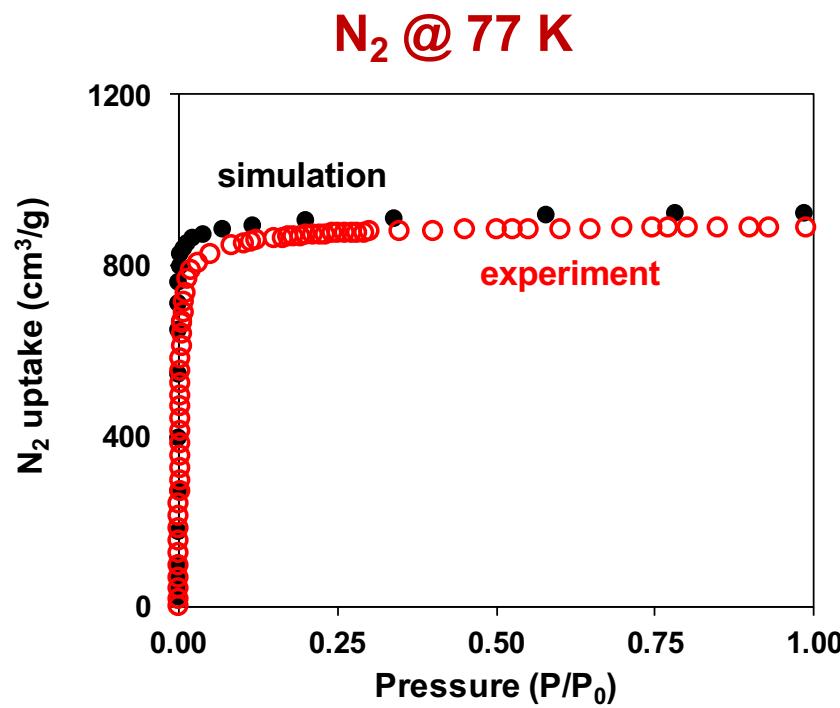
UMCM-152



Journal of the American Chemical Society, 2010, 132, 13941

Nature Communications 2018, 9, 1378

Experiments Successfully Confirm Predictions

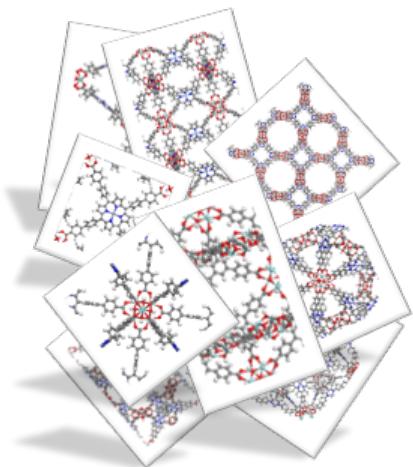


Synthesised sample is highly crystalline and successfully activated

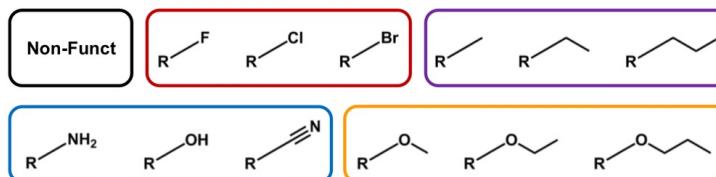
UMCM-152 delivers 22.5% more oxygen than NU-125 and 90% more than empty tank

Computer-aided Discovery of MOFs for Adsorption Applications

High-throughput screening of a large number of MOFs

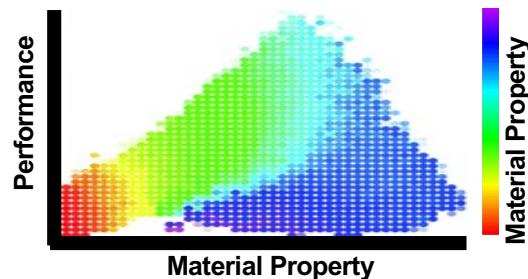


Identify **Design Rules** for the desired storage application



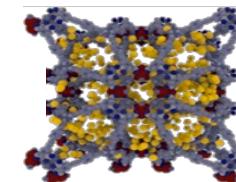
Structure-Property relationships

e.g. Pore size, surface area, framework density

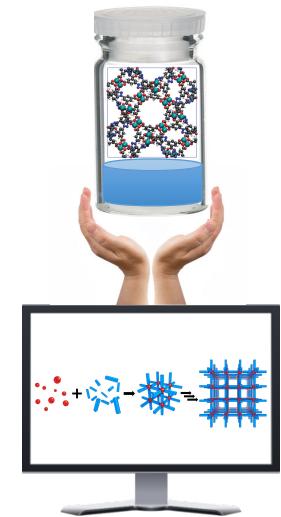


Identify outstanding materials; In depth study of performance over process conditions

GCMC and Quantum Mechanical Calculations



Laboratory synthesis of top-performing MOFs



Increased Computational Time

Acknowledgements

CCDC

Dr. Jason Cole
Dr. Seth Wiggin
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Northwestern University

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Prof. Omar Farha
Prof. Fraser Stoddart

Shell

Marcel Dabkowski
Pim Mul

Svante

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Carl McGrath



Engineering and Physical Sciences
Research Council



Innovate UK



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14 October 2021