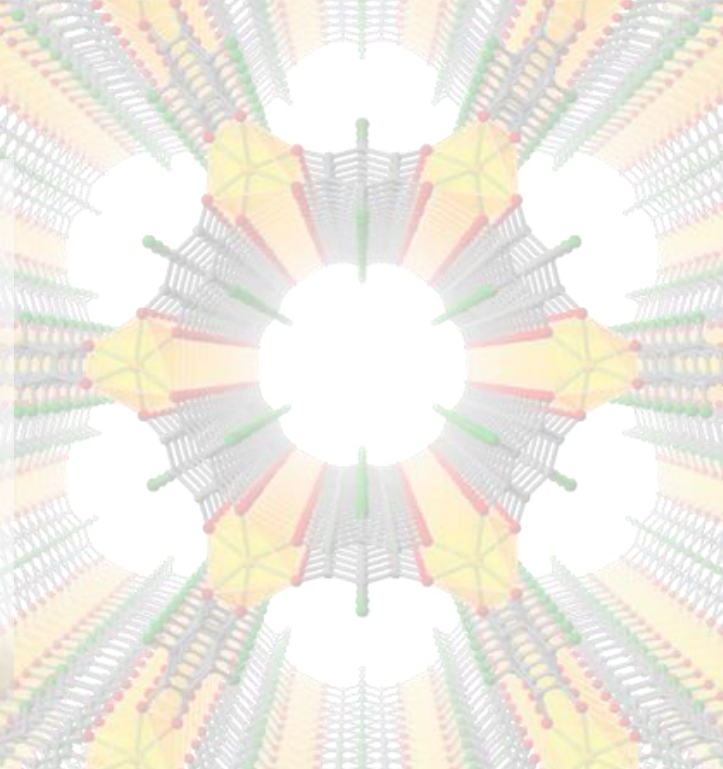


Magforming Chemistry: From Methane Capture to Hydrogen Storage



Lujia (Luke) Liu, Lecturer in Inorganic Chemistry
Nelson, 7 December 2022

As A Magnetochemist...

The screenshot shows an Amazon product page for the Magformers Basic Set (30 pieces) magnetic building blocks. The page includes the Amazon logo, delivery location (New Zealand), search bar, navigation menu, and product details. The product is priced at \$40.13, a 20% discount from the list price of \$49.99. It features 30 pieces of colorful magnetic building blocks that can be used to create various geometric shapes like a cube, a pyramid, and a dodecahedron. The product has a 4.5-star rating from 3,640 ratings and 82 answered questions.

amazon Deliver to New Zealand All magformers

Today's Deals Customer Service Registry Gift Cards Sell

Toys & Games Holiday Toy List Shop by Age Shop Toys by Character Shop Best Selling Toys Shop Newly Released Toys Shop Amazon Exclusive Toys Shop Toy Deals Create a Birthday Gift List Create a Holiday Gift List

Save 39% Savings & Sales Magblock Magnetic Tiles Pipe Magnetic... 4.2/5 (4,278 ratings) \$42.49 \$69.99 Prime

Back to results

MAGFORMERS BASIC 30 PCS 3+ AGE

Magformers Basic Set (30 pieces) magnetic building blocks, educational magnetic tiles, magnetic building STEM toy - 63076 , Rainbow

Visit the Magformers Store

4.5/5 (3,640 ratings) | 82 answered questions

List Price: \$49.99
Price: \$40.13
You Save: \$9.86 (20%)

No Import Fees Deposit & \$13.99 Shipping to New Zealand Details

Sales taxes may apply at checkout

Available at a lower price from other sellers that may not offer free Prime shipping.

Extra Savings 50% off gift wrap service: code GIFT... 1 Applicable Promotion

Brand	Magformers
Age Range (Description)	Magformers are recommended for children ages 3 and older.
Model Name	63076
Theme	Floral
Material	Neodymium rare-earth magnets for guaranteed connectivity.
Number of Pieces	30

See more

Magformers Basic Set (30 pieces) magnetic building blocks, educational magnetic tiles, magnetic building STEM toy - 63076 , Rainbow

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See more

About this item

- Set contains the exact number required to build the classic magic ball
- Made with high quality and super powerful magnets
- Makes a great add-on to any MAGFORMERS collection
- Perfect set for traveling, because the pieces stick together
- An educational experience that's also fun

Magforming Polyhedrons



Tetrahedron

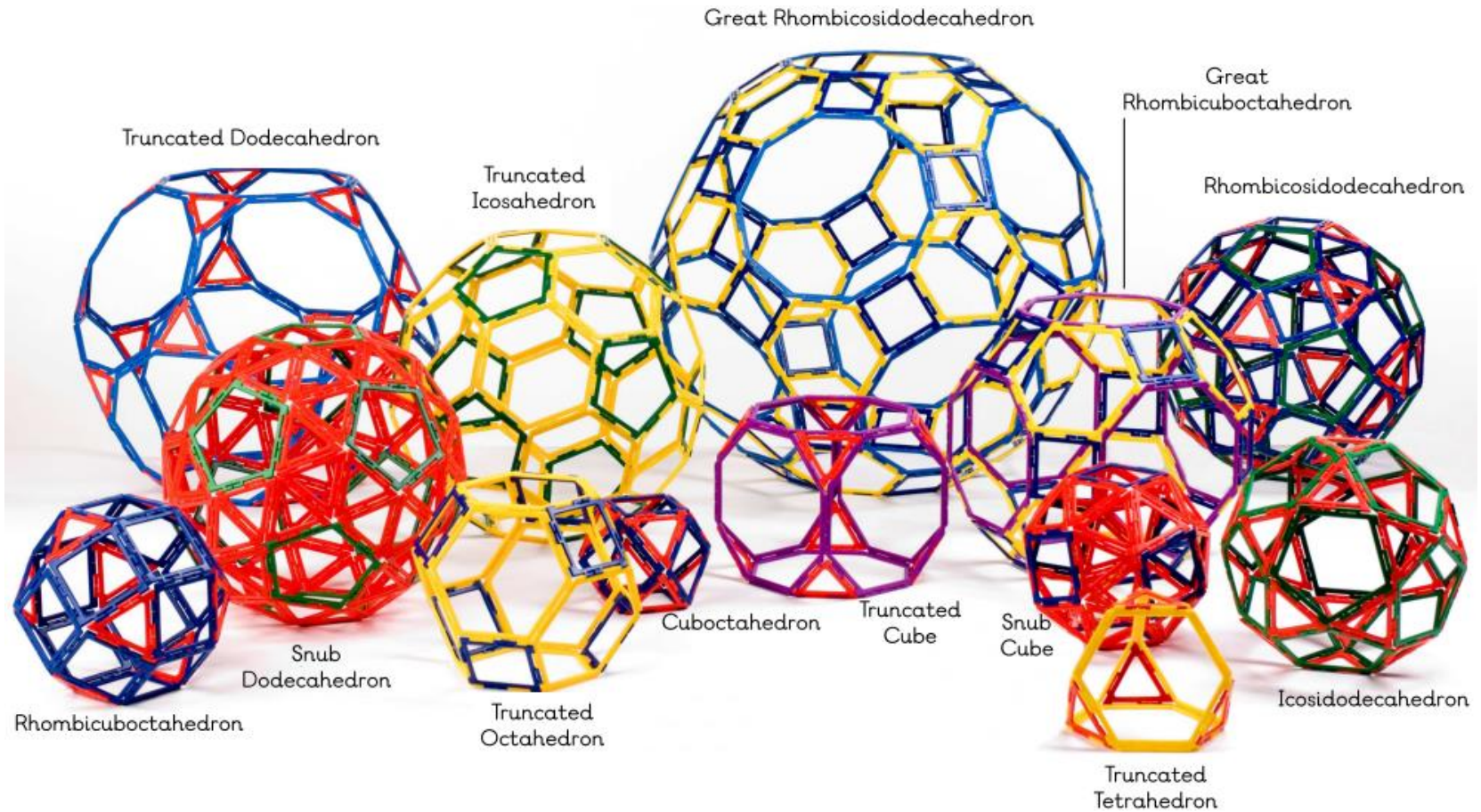
Cube

Octahedron

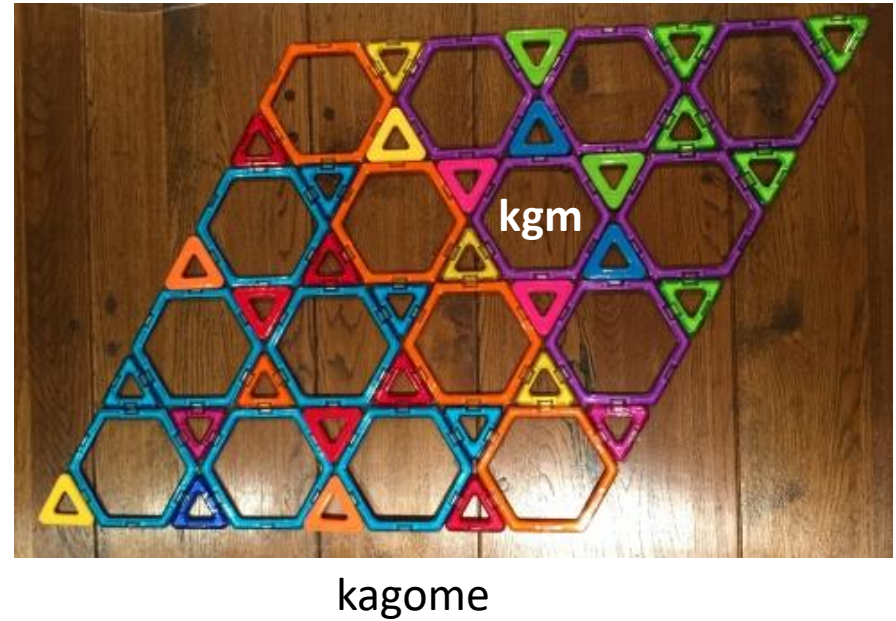
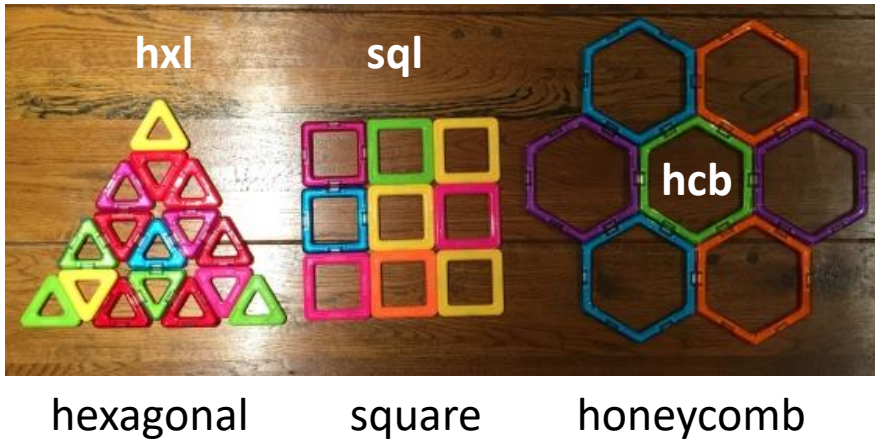
Icosahedron

Dodecahedron

Magforming Polyhedrons



Magforming 2D Lattices



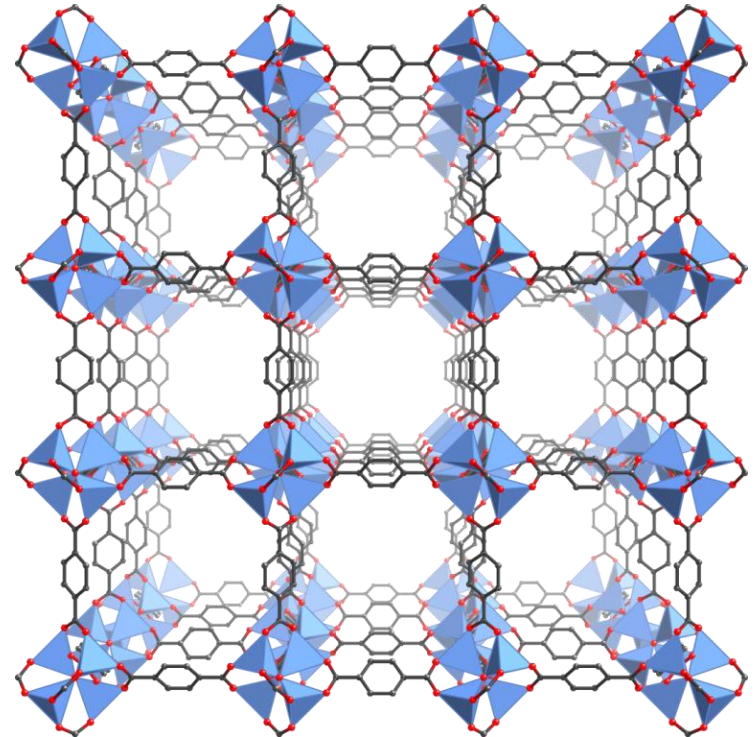
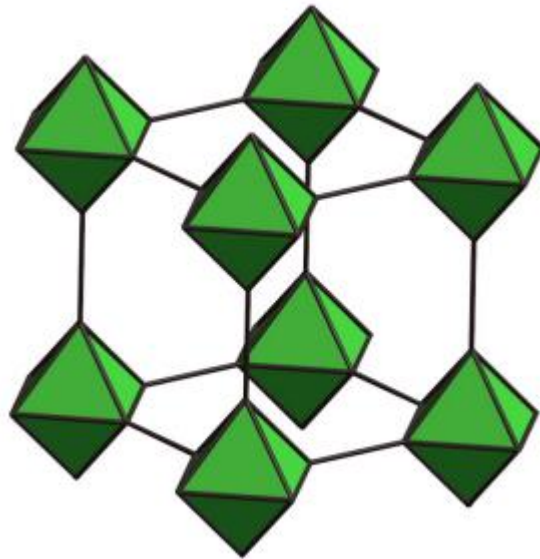
**CAPITAL THINKING.
GLOBALLY MINDED.**
MAI I TE IHO KI TE PAE



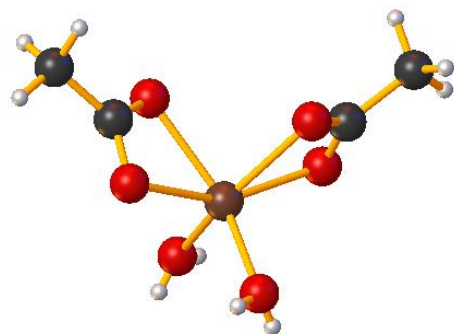
VICTORIA UNIVERSITY OF
WELLINGTON
TE HERENGA WAKA

Magforming 3D Lattices

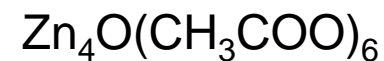
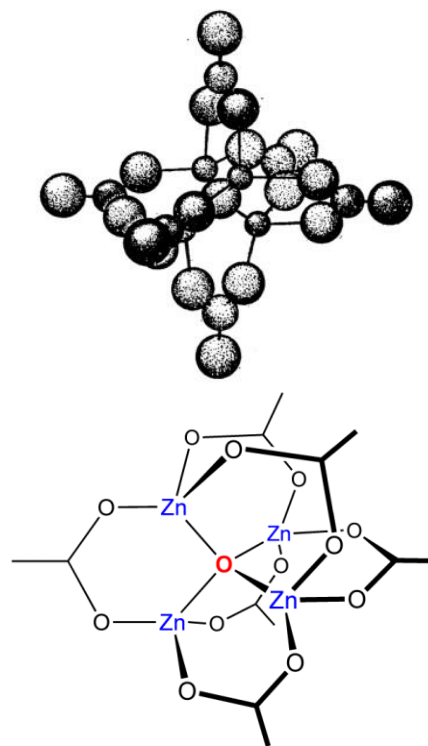
Linking octahedron to form **pcu** (primitive cubic) network



Octahedron Chemical Building Block



Sublimation



H. Koyama & Y. Saito; The Crystal Structure of Zinc Oxyacetate, $\text{Zn}_4\text{O}(\text{CH}_3\text{COO})_6$. *Bull. Chem. Soc. Jpn.* **1954**, 27, 112-114.

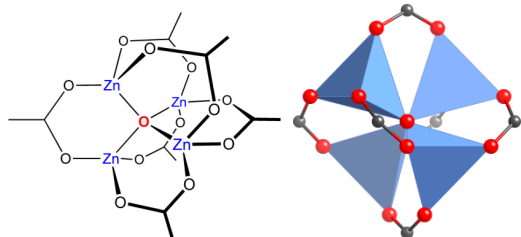
Metal-Organic Framework-5 (MOF-5)



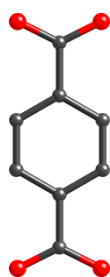
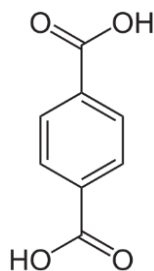
III

+

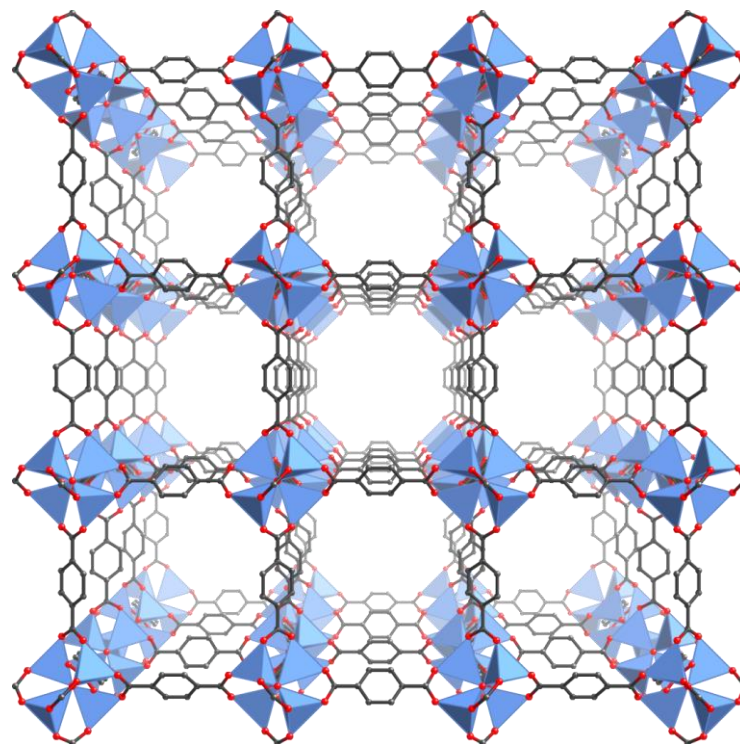
III



$Zn_4O(CO_2-R)_6$ cluster



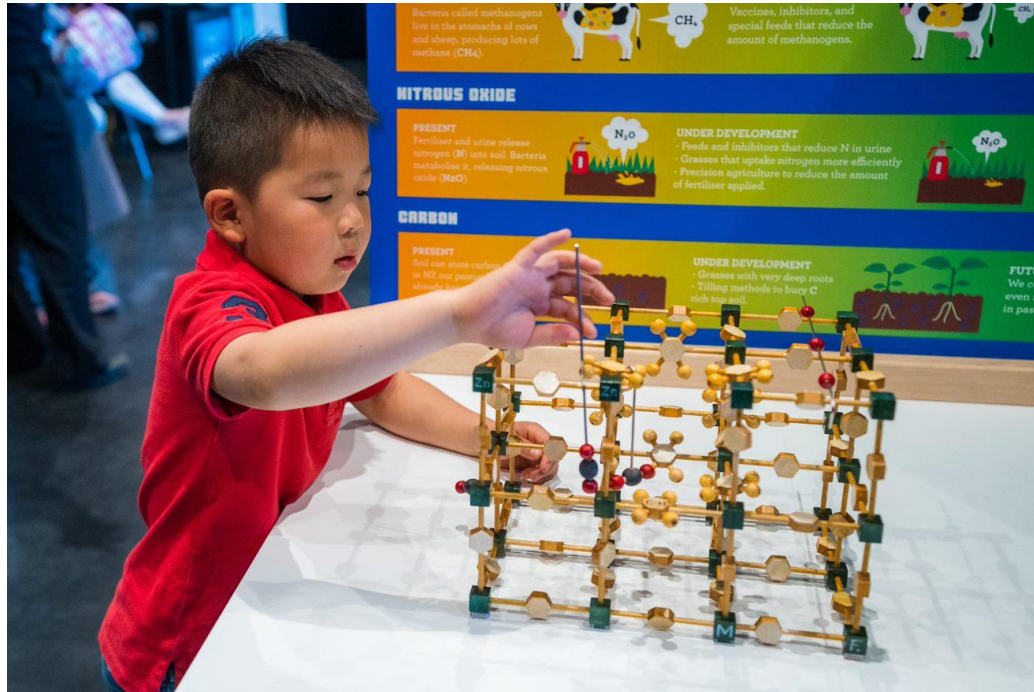
Terephthalic acid
 H_2BDC



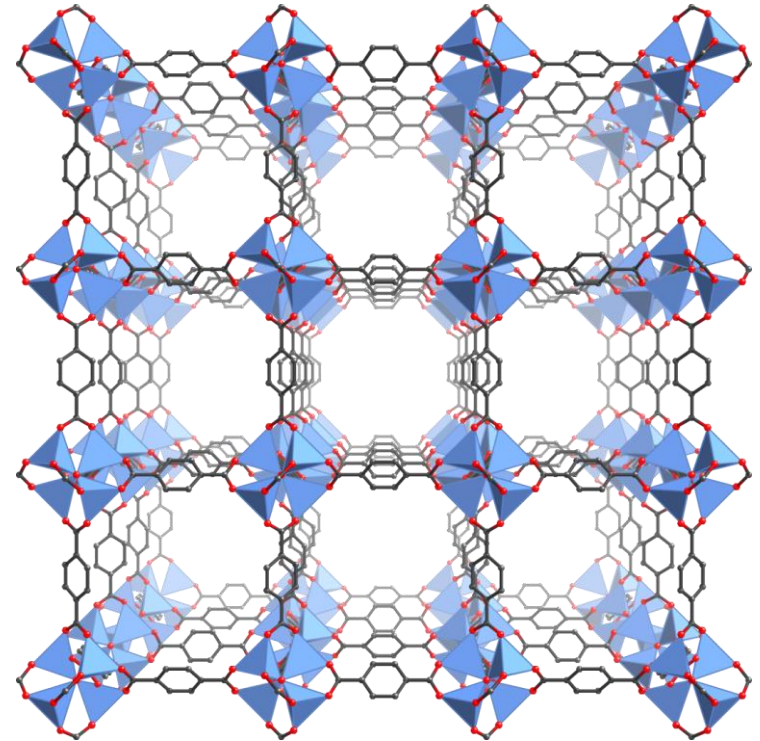
MOF-5 [$Zn_4O(BDC)_3$]
Surface Area = 3500 m²/g

H. Li, M. Eddaoudi, M. O'Keeffe, O. M. Yaghi, *Nature*, **1999**, 402, 276-279.

Metal-Organic Framework-5 (MOF-5)



MOF-5 Model at Otago Museum
(Te Papa also has a MOF-5 model)

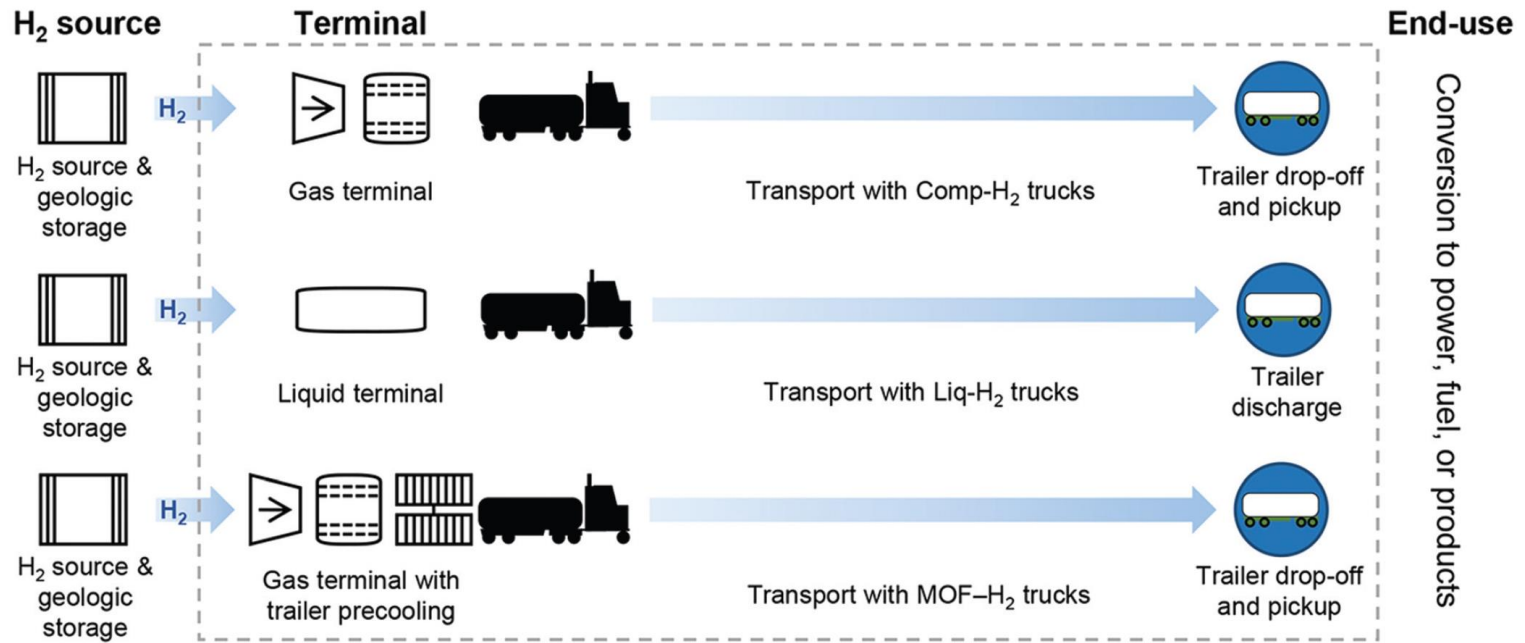


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MOF-5 for Hydrogen Storage

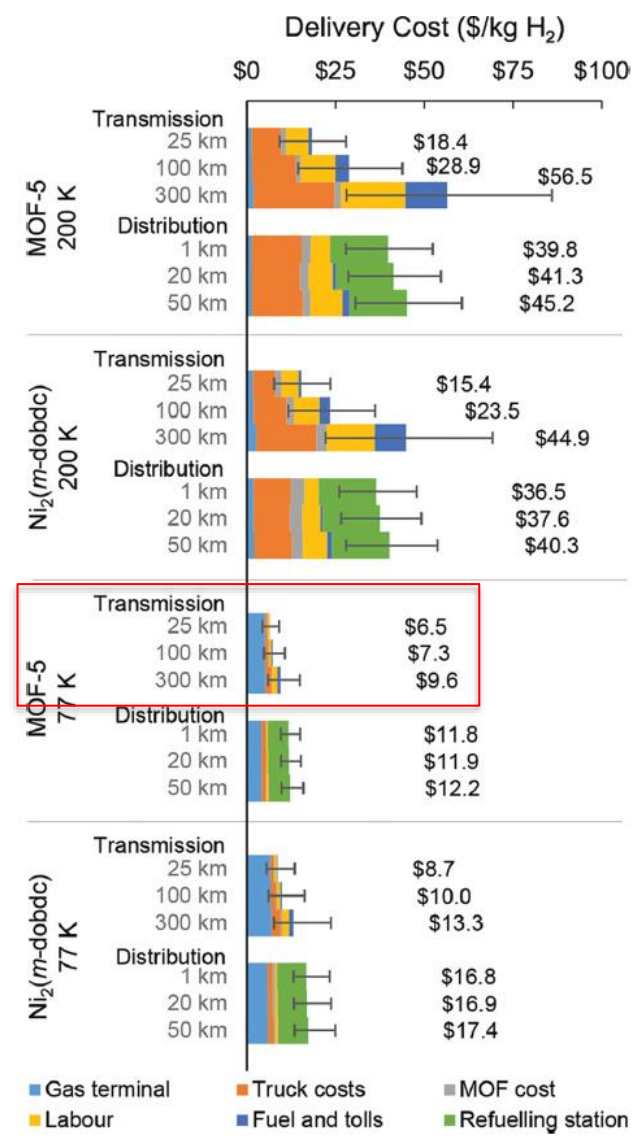
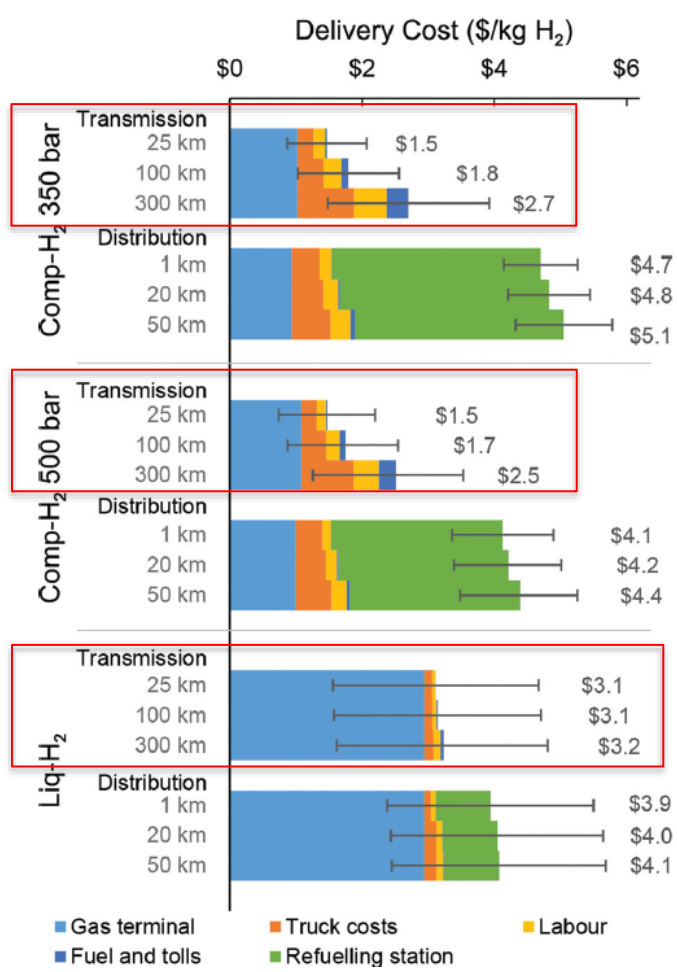
System boundaries for long-distance transmission



Yaghi and co-workers, *Science* **2003**, 300, 1127.

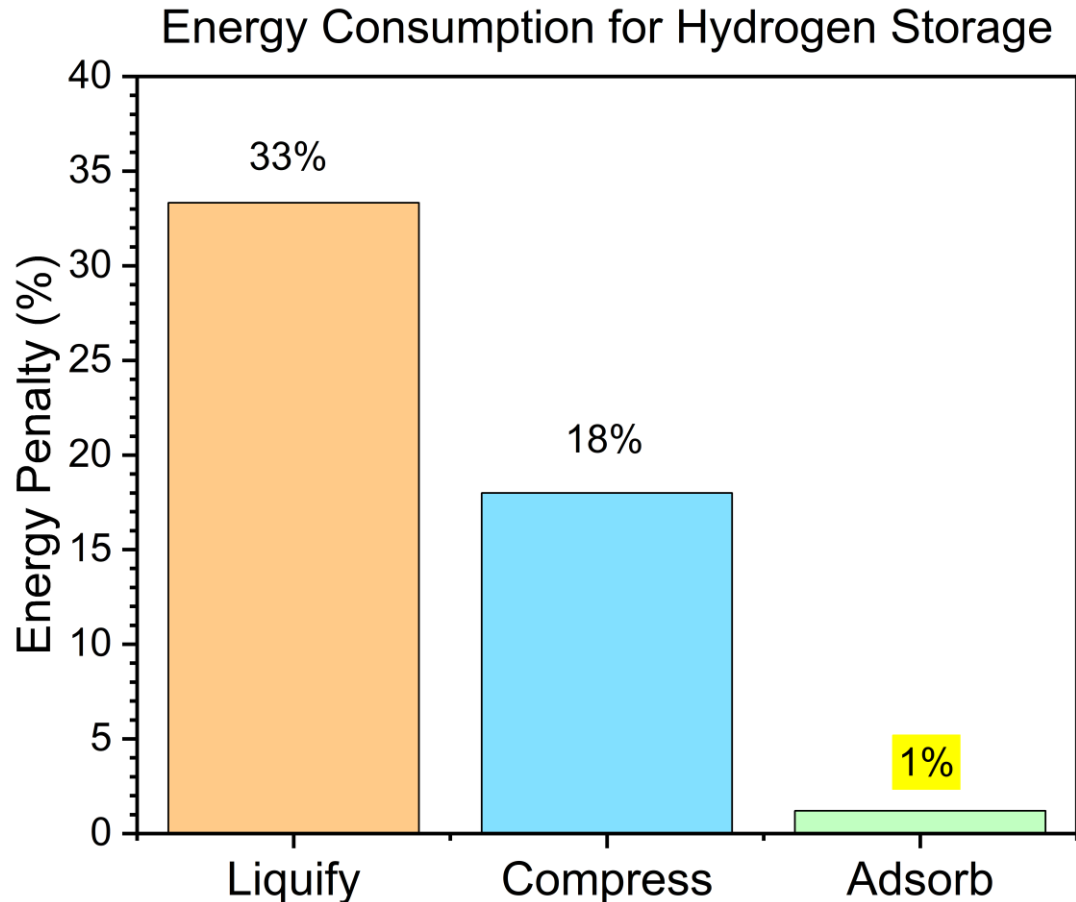
Matzger and co-workers, *Nat. Commun.*, **2019**, 10, 1568.

Breunig, Long and co-workers, *Energy Environ. Sci.*, **2021**, 14, 1083.

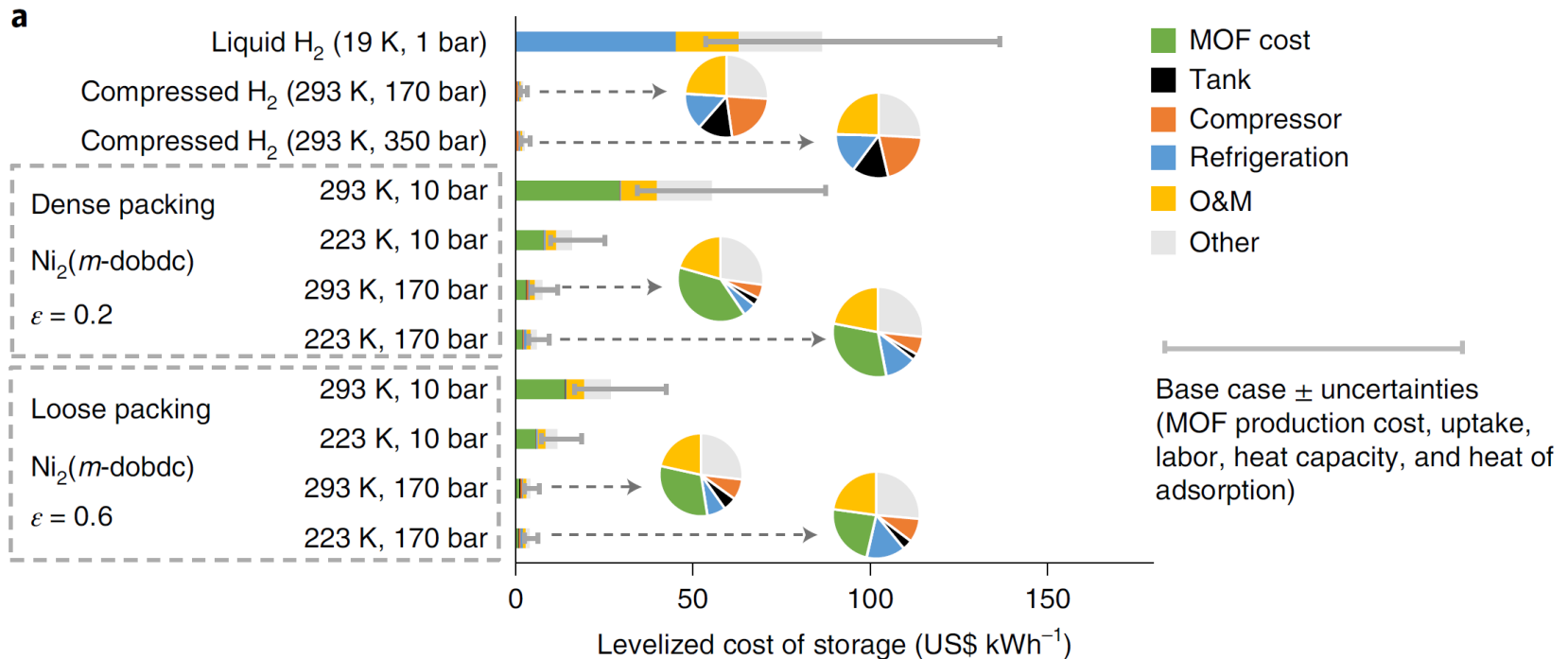


Breunig, Long and co-workers, *Energy Environ. Sci.*, 2021, 14, 1083.

Why MOFs for Hydrogen Storage?



Hydrogen Storage MOFs for Back-up Power Supply



Breunig, Long and co-workers, *Nature Energy*, 2022, 7, 448.

Further Cost Reduction?

- Increase Materials Durability
- Increase Storage Capacity

How?

Methane Emissions



Methane is 25× more potent greenhouse gas than CO₂ (100-year span).

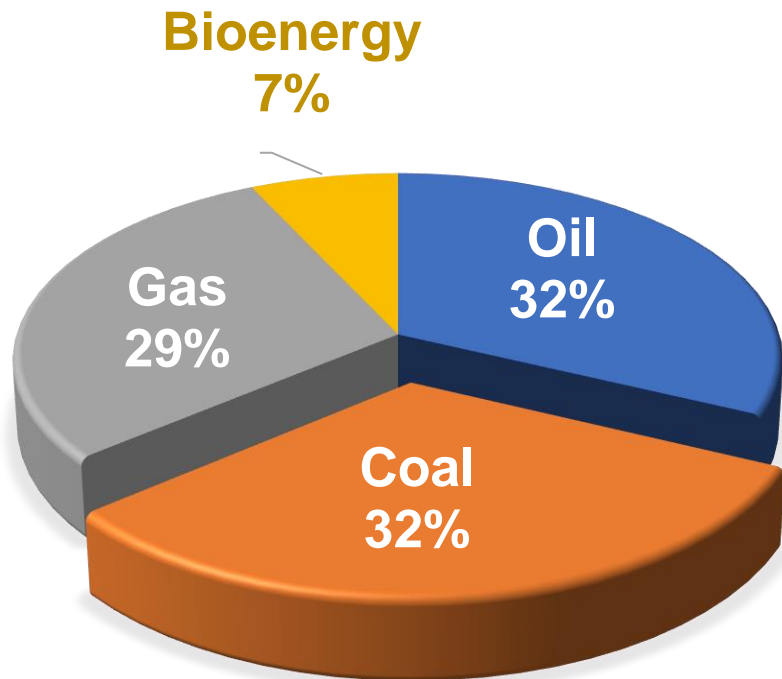


Methane emissions' contribution to global warming:
20% -- US Environment Protection Agency
30% -- International Energy Agency



The **energy sector** is responsible for 38% of human-activity-related emissions, second only to agriculture (40%).

Methane Emissions by The Energy Sector

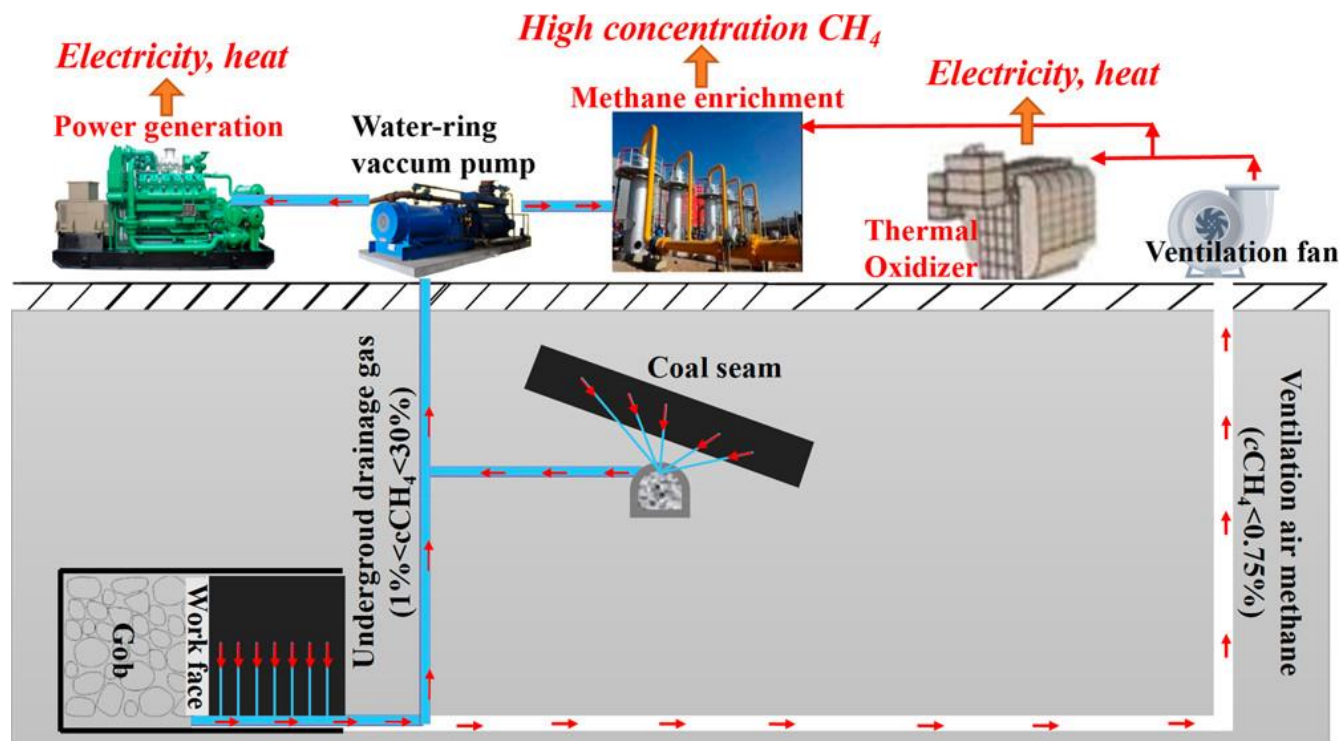




Flaring



Explosion limit: 5 – 15 % in air

Coal Mine Methane Capture



-  Drainage gas (methane $> 6\%$) utilisation rate reached 45% in China (2020).
-  Capturing ventilation air methane (methane $< 0.75\%$) remains a challenge.

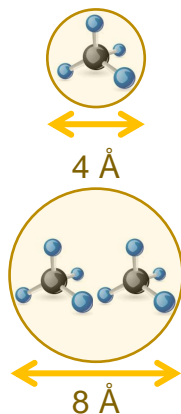
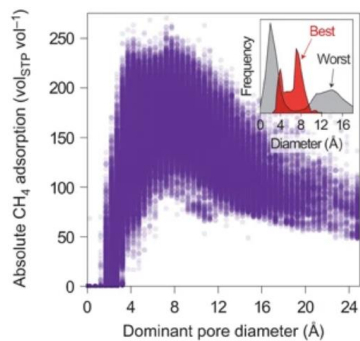
Design Principles for Methane Capture Materials



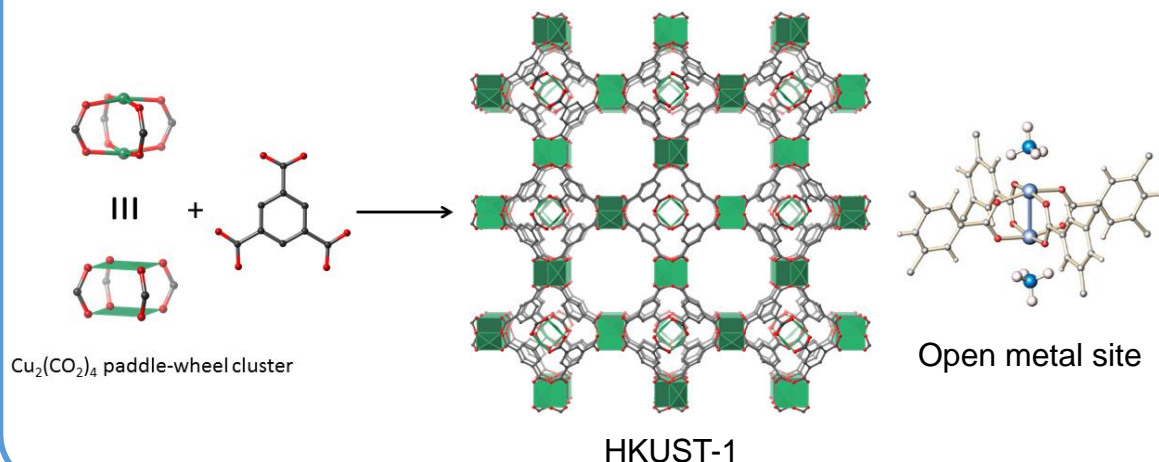
Selective for CH₄ over other gases in the air (mostly N₂)

Gas	Kinetic Diameter (Å)	Polarisability (Å ³)
CH ₄	3.80	2.6
N ₂	3.64	1.4

Simulations over 137,000 hypothetical MOFs



MOFs with open metal sites show higher CH₄/N₂ selectivity



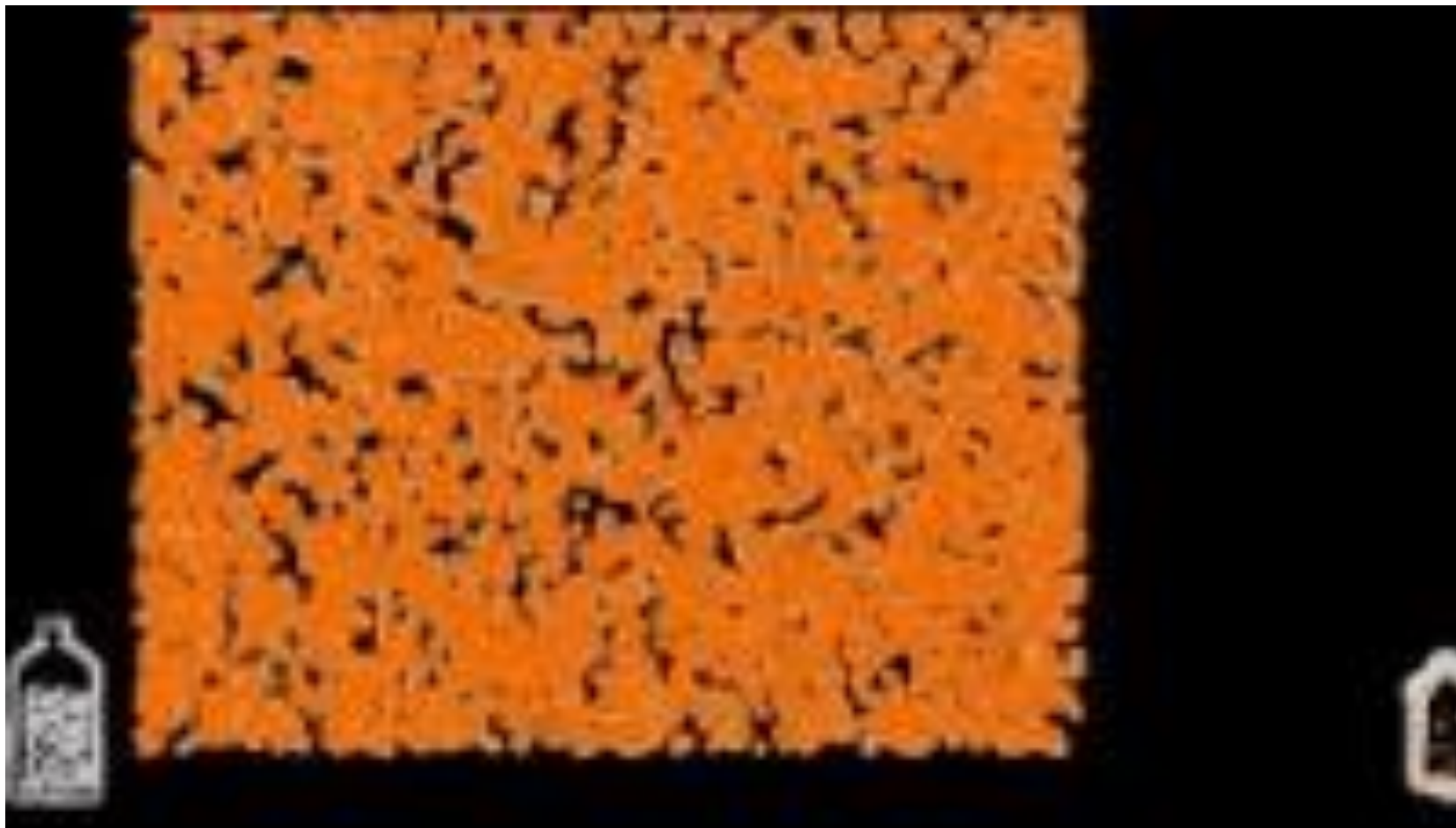
R. Q. Snurr and co-workers, *Nature Chem.* **2011**, *4*, 83.

I. D. Williams and co-workers, *Science* **1999**, *283*, 1148.

Wei Zhou and co-workers, *J. Am. Chem. Soc.* **2009**, *131*, 4995.

O. K. Farha and co-workers *J. Am. Chem. Soc.* **2013**, *135*, 11887.

Simulations over 137,000 hypothetical MOFs



https://www.youtube.com/watch?v=bVVvTH_d4hl

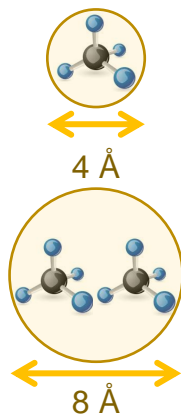
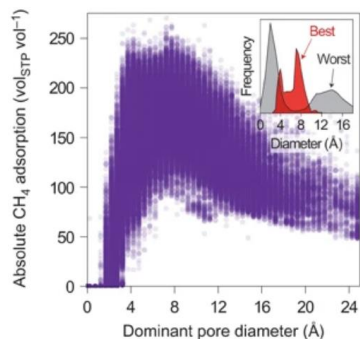
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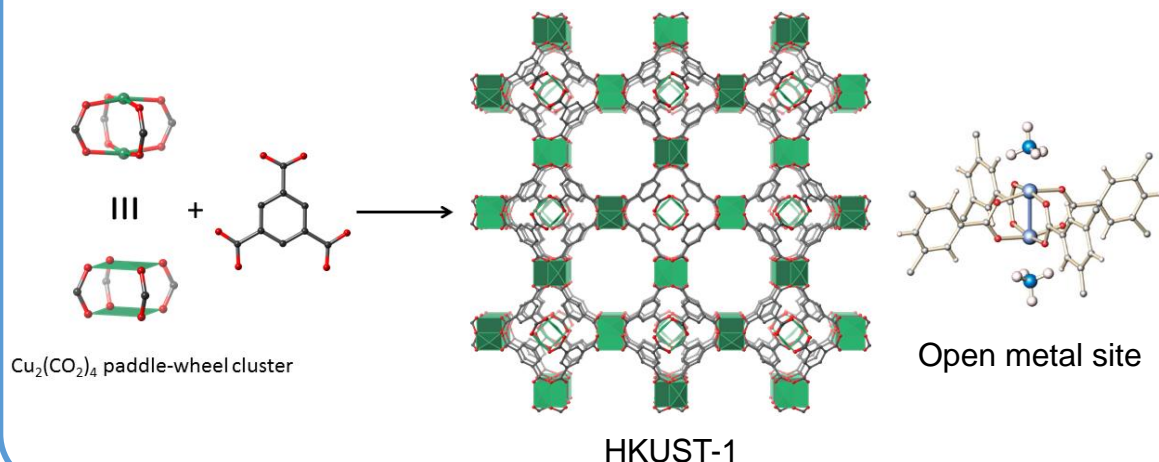
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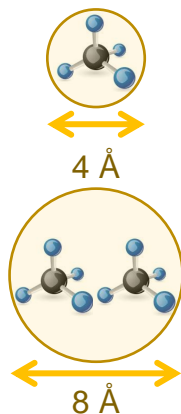
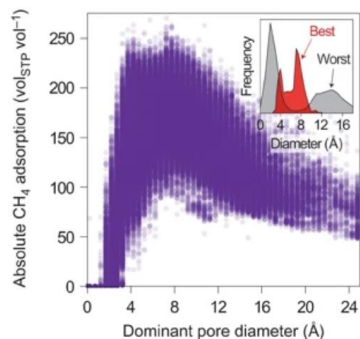
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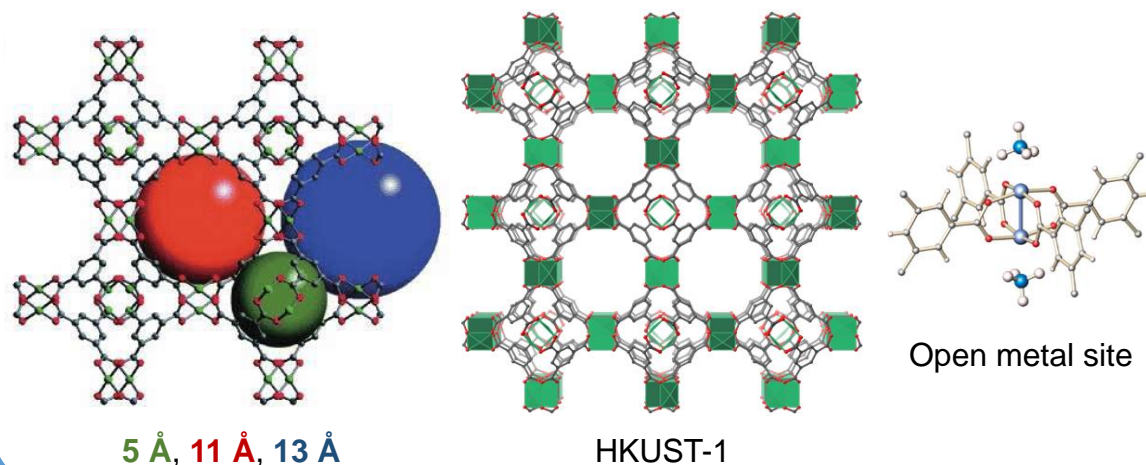
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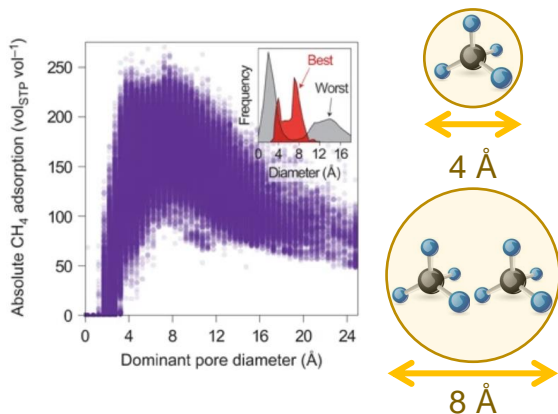
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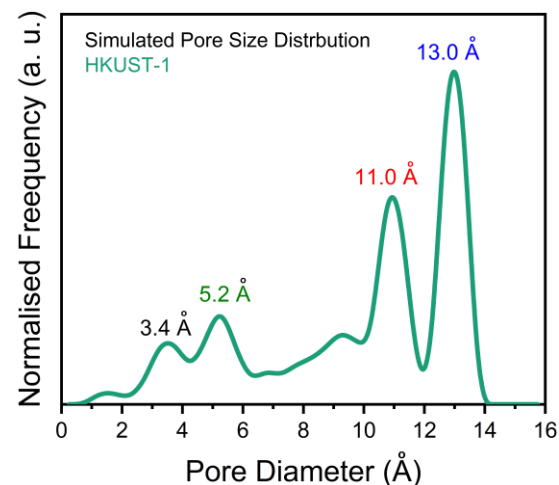
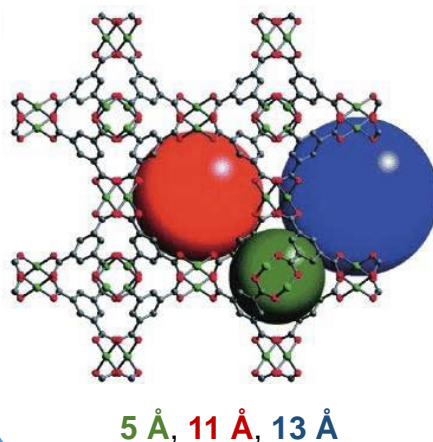
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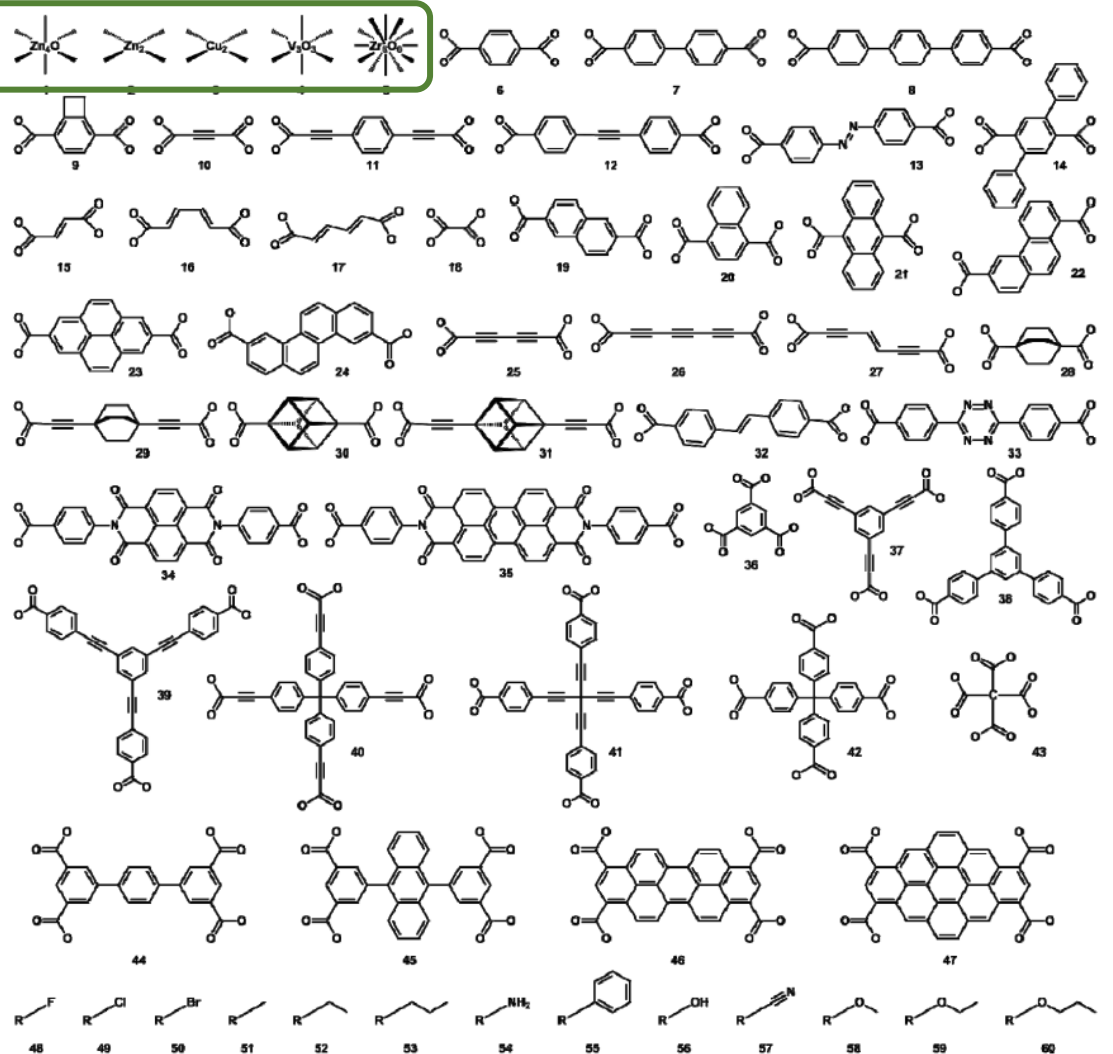
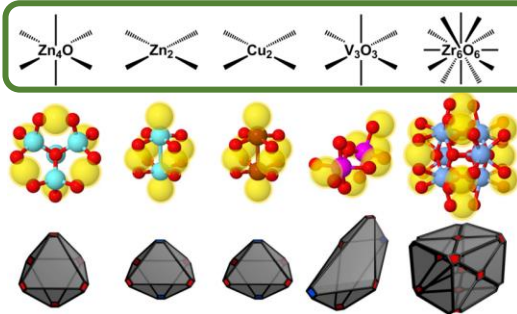
O. K. Farha and co-workers *J. Am. Chem. Soc.* **2013**, *135*, 11887.

Our Goal

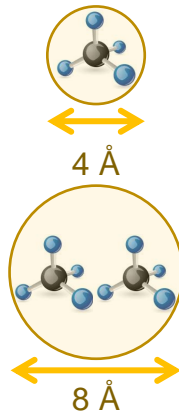
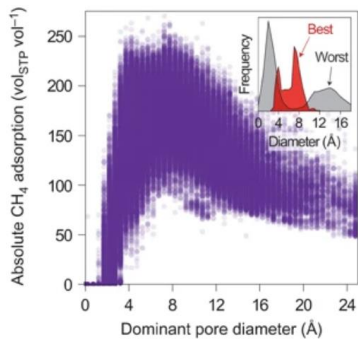
Design a material with **both** open metal sites and optimal pore sizes

Our Goal

Design materials with **both** open metal site and optimal pore size


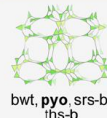

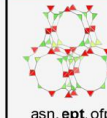
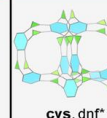
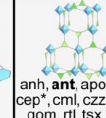

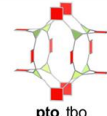
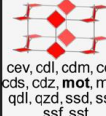
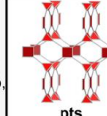
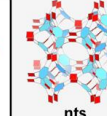
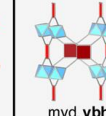

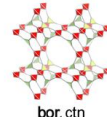
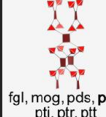
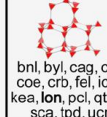
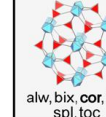
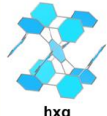
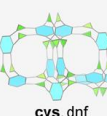
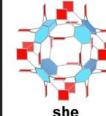
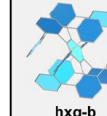
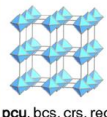

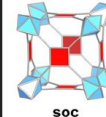
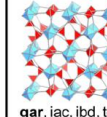
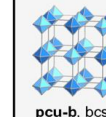
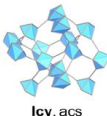

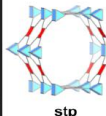
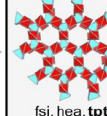
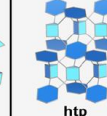
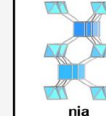


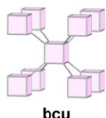
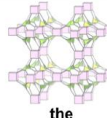
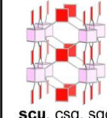
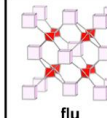
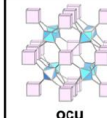
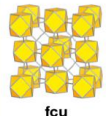
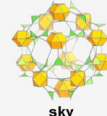
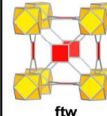
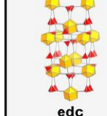
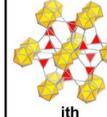
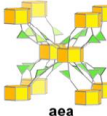
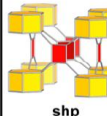
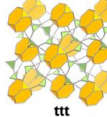
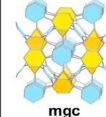
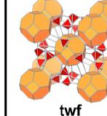
Simulations over 137,000 hypothetical MOFs



Our Goal

Design a material with **both** open metal sites and **optimal** pore sizes

Building unit 1 \ Building unit 2	2-c Linear	3-c Triangle	4-c Square	4-c tet	6-c Hexagon	6-c oct
3-c Triangle	 srs	 bwt, pyo, srs-b, ths-b	 fjh, fmj, gee, iab, yac, yao	 asn, ept, ofp	 cys, dnf*	 anh, ant, apo, brk, cep*, cml, czz, eea, qom, rtl, tsx, zzz
4-c Square	 nbo, lvt, rhr	 pto, tbo	 cev, cdl, cdm, cdu, cds, cdz, mot, muo, qdl, qzd, ssd, sse, ssf, sst	 pts	 nts	 myd, ybh
4-c tet	 dia, lcs, qtz, sod	 bor, ctn	 fgl, mog, pds, pth, pti, ptr, ptt	 bnl, byl, cag, cbt, coe, crb, fel, icm, kea, lon, pcl, qtz-b, sca, tpd, ucn	-	 alw, bix, cor, ing, spl, toc
6-c Hexagon	 hxg	 cys, dnf	 she	-	 hxg-b	-
6-c oct	 pcu, bcs, crs, reo	 pyr, spn	 soc	 gar, iac, ibd, toc	-	 pcu-b, bcs-b
6-c trp	 lcy, acs	 ceq, dag, fmz, hwx, moo, sab, sit, ydq	 stp	 fsi, hea, tpt	 htp	 nia

Building unit 1 \ Building unit 2	2-c Linear	3-c Triangle	4-c Square	4-c tet	6-c Hexagon	6-c oct
8-c cub	 bcu	 the	 scu, csq, sqc	 flu	-	 ocu
12-c cuo	 fcu	 sky	 ftw	 edc	-	-
12-c ico	-	-	-	 ith	-	-
12-c hpr	-	 aea	 shp	-	-	-
12-c tte	-	 ttt	-	-	 mgc	-
24-c tro	-	-	-	 twf	-	-

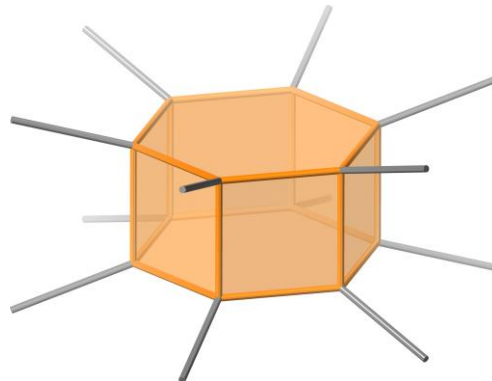
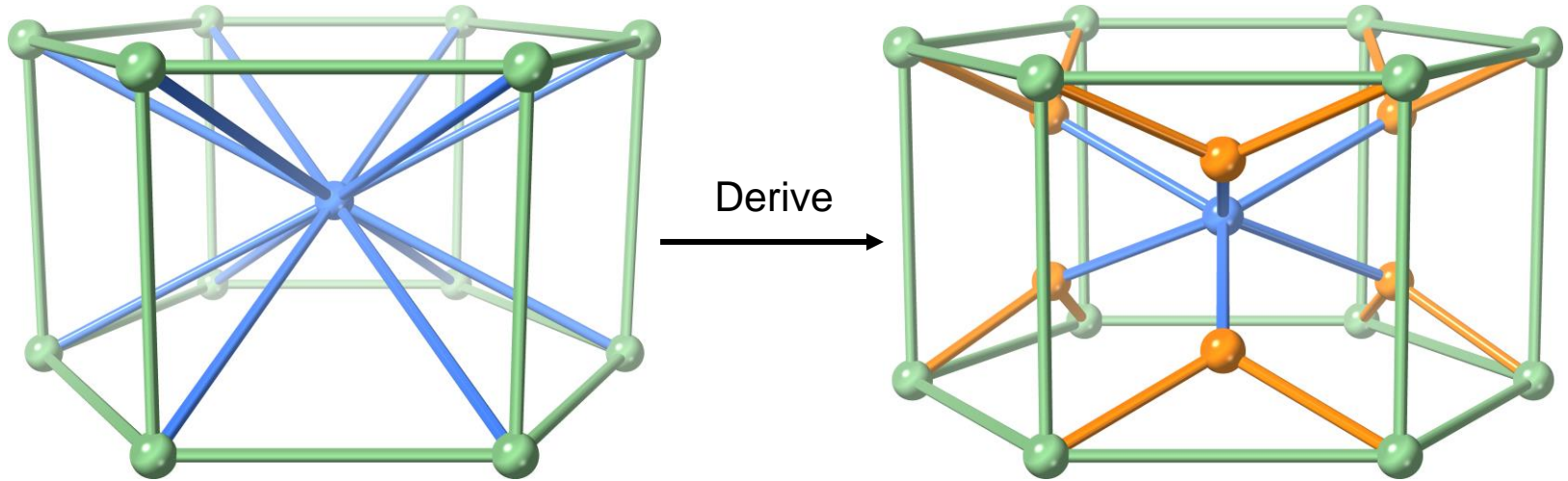
Our Goal

Design a material with **both** open metal sites and optimal pore sizes

Building unit 1 \ Building unit 2	2-c Linear	3-c Triangle	4-c Square	4-c tet	6-c Hexagon	6-c oct
3-c Triangle	srs	bwt, pyo, srs-b, ths-b	fjh, fmj, gee, iab, yac, yao	asn, ept, ofp	cys, dnf*	anh, ant apo, brk, cep*, cml, czz, eea, qom, rtl, tsx, zzz
4-c Square	nbo, lvt, rhr	pto, tbo	cev, cdl, cdm, cdu, cds, cdz, mot, muo, qdl, qzd, ssd, sse, ssf, sst	pts	nts	myd, ybh
4-c tet	dia, lcs, qtz, sod	bor, ctn	fgl, mog, pds, pth, pti, ptr, ptt	bnl, byl, cag, cbt, coe, crb, fel, icm, kea, lon, pcl, qtz-b, sca, tpd, ucn	-	alw, bix, cor, ing, spl, toc
6-c Hexagon	hxg	cys, dnf	she	-	hxg-b	-
6-c oct	pcu, bcs, crs, reo	pyr, spn	soc	gar, iac, ibd, toc	-	pcu-b, bcs-b
6-c trp	lcy, acs	ceq, dag, fmz, hwx, moo, sab, sit, ydq	stp	fsi, hea, tpt	htp	nia

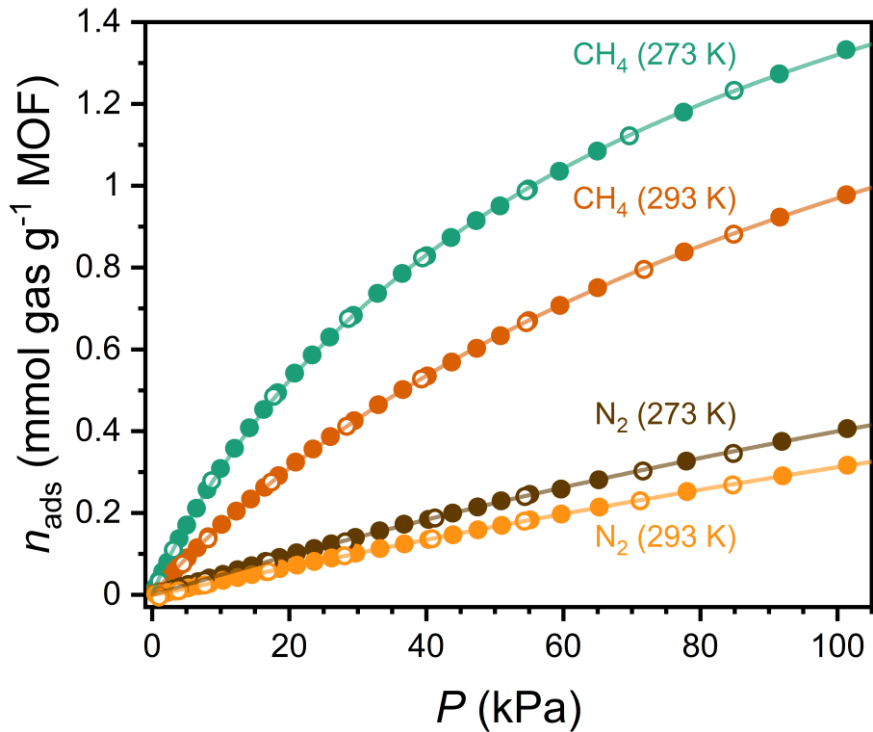
Building unit 1 \ Building unit 2	2-c Linear	3-c Triangle	4-c Square	4-c tet	6-c Hexagon	6-c oct
8-c cub	bcu	the	scu, csq, sqc	flu	-	ocu
12-c cuo	fcu	sky	ftw	edc	-	-
12-c ico	-	-	-	ith	-	-
12-c hpr	-	aea	shp	-	-	-
12-c tte	-	ttt	-	-	mgc	-
24-c tro	-	-	-	twf	-	-

Deriving The 12-c Building Block

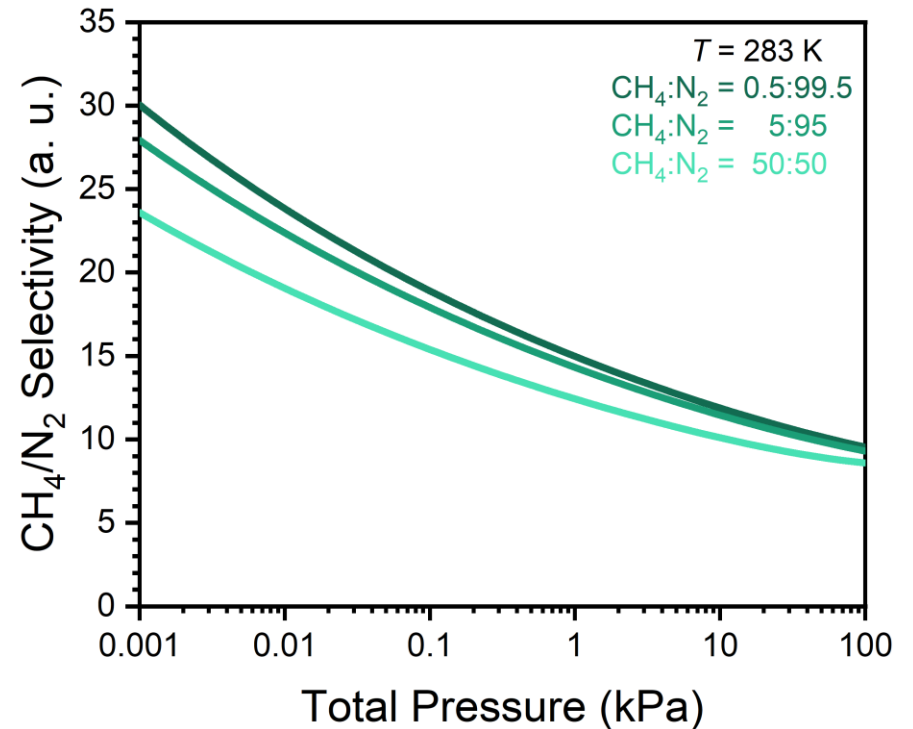


Methane Capture Performance

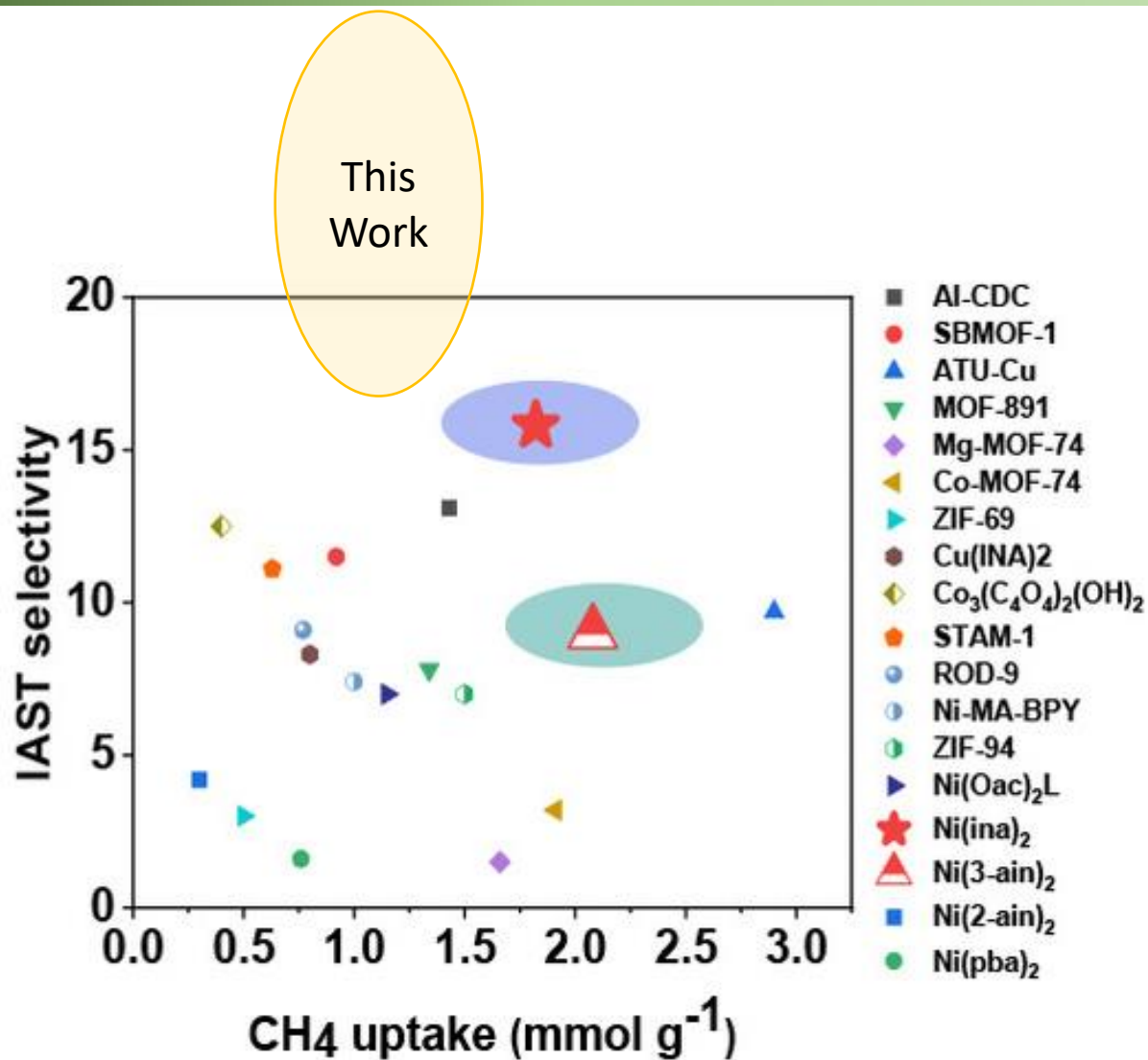
Adsorption isotherms



CH_4/N_2 Selectivity



CH₄/N₂ Selectivity Comparison



Further Cost Reduction for Hydrogen Storage?

- Increase Materials Durability
- Increase Storage Capacity

How?

Further Cost Reduction for Hydrogen Storage?

- Increase Materials Durability
- Increase Storage Capacity

How?

- Increase Materials Durability – Stronger Bonds
- Increase Storage Capacity – Higher Surface Area

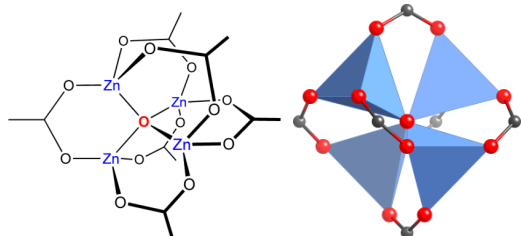
Metal-Organic Framework-5 (MOF-5)



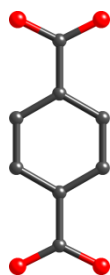
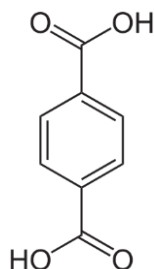
III

+

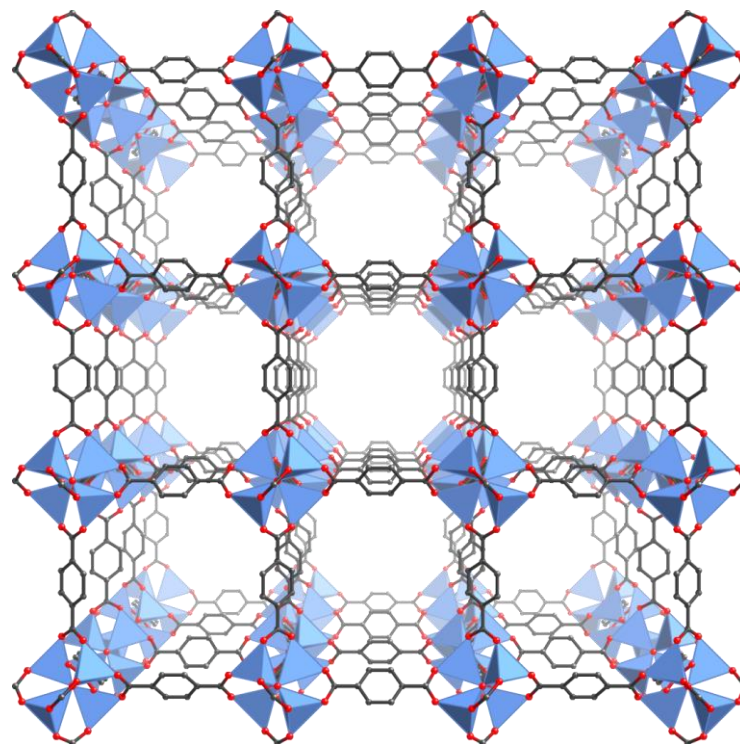
III



$Zn_4O(CO_2-R)_6$ cluster



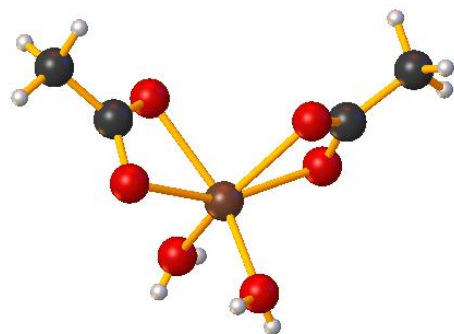
Terephthalic acid
 H_2BDC



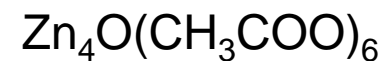
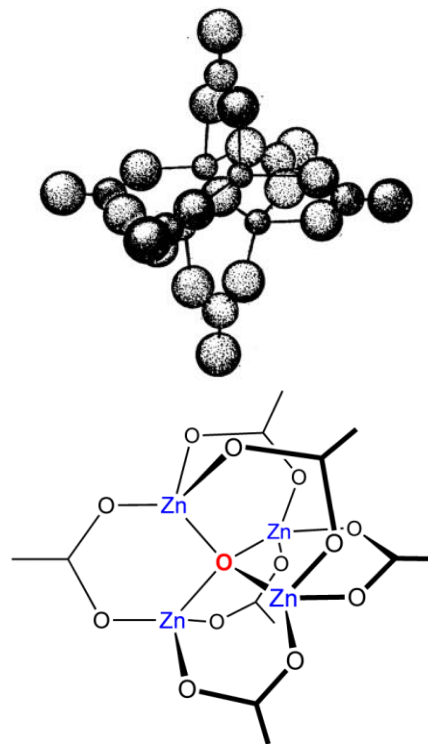
MOF-5 [$Zn_4O(BDC)_3$]
Surface Area = 3500 m²/g

H. Li, M. Eddaoudi, M. O'Keeffe, O. M. Yaghi, *Nature*, **1999**, 402, 276-279.

Octahedron Chemical Building Block

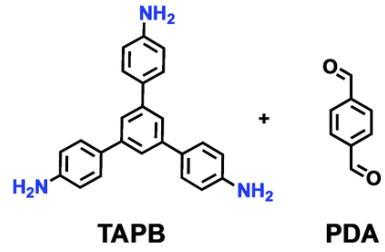
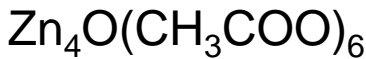
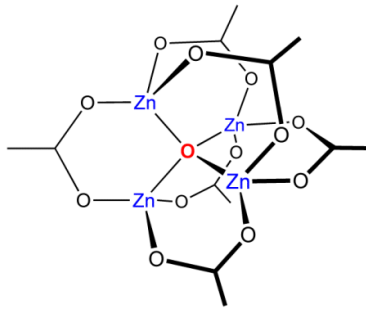


Sublimation

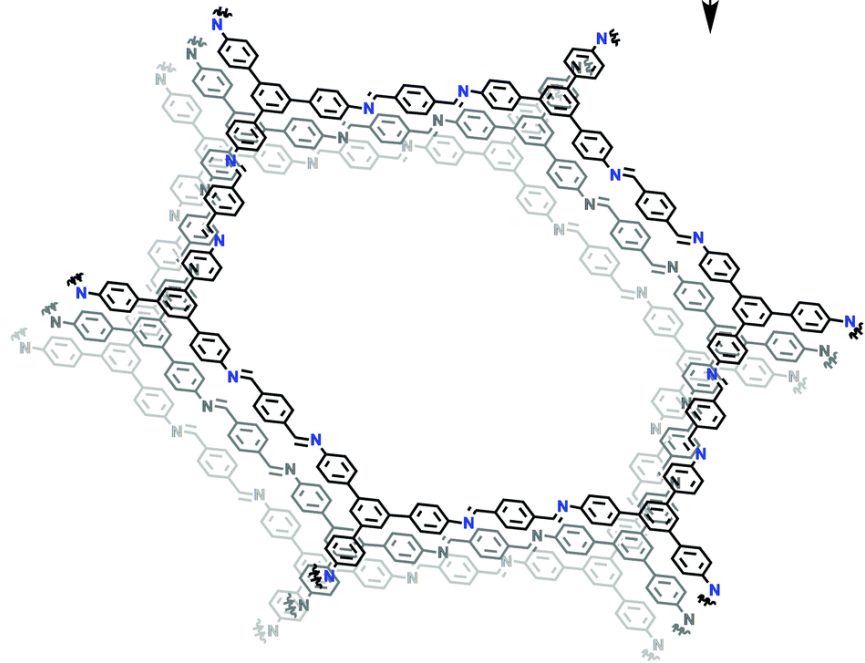
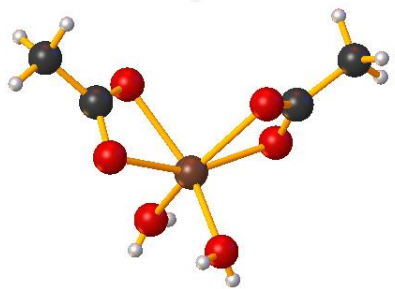


H. Koyama & Y. Saito; The Crystal Structure of Zinc Oxyacetate, $\text{Zn}_4\text{O}(\text{CH}_3\text{COO})_6$. *Bull. Chem. Soc. Jpn.* **1954**, 27, 112-114.

From Weaker Coordination Bonds to Stronger Covalent Bonds

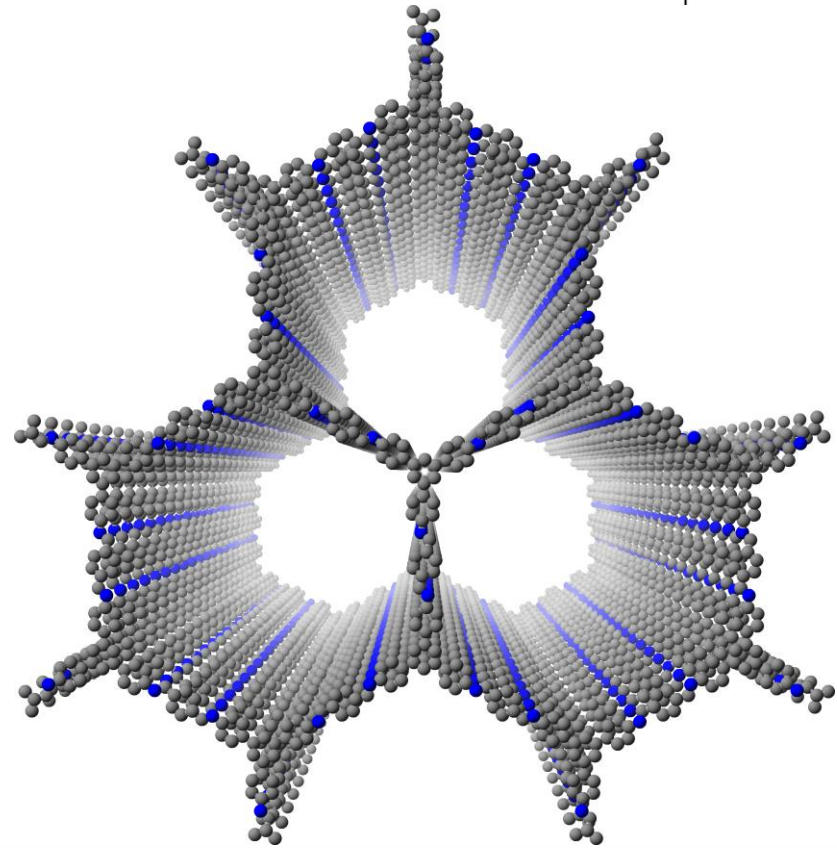
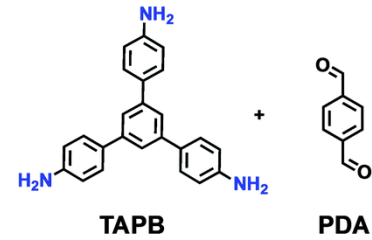
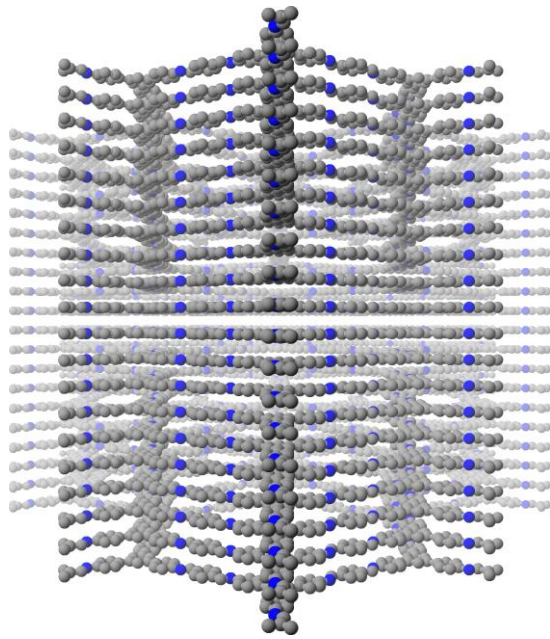


> 30%
Relative Humidity



Covalent organic frameworks (COFs)

Covalent organic frameworks



honeycomb

Further Cost Reduction for Hydrogen Storage?

- Increase Materials Durability
- Increase Storage Capacity

How?

- Increase Materials Durability – Stronger Bonds
- Increase Storage Capacity – Higher Surface Area

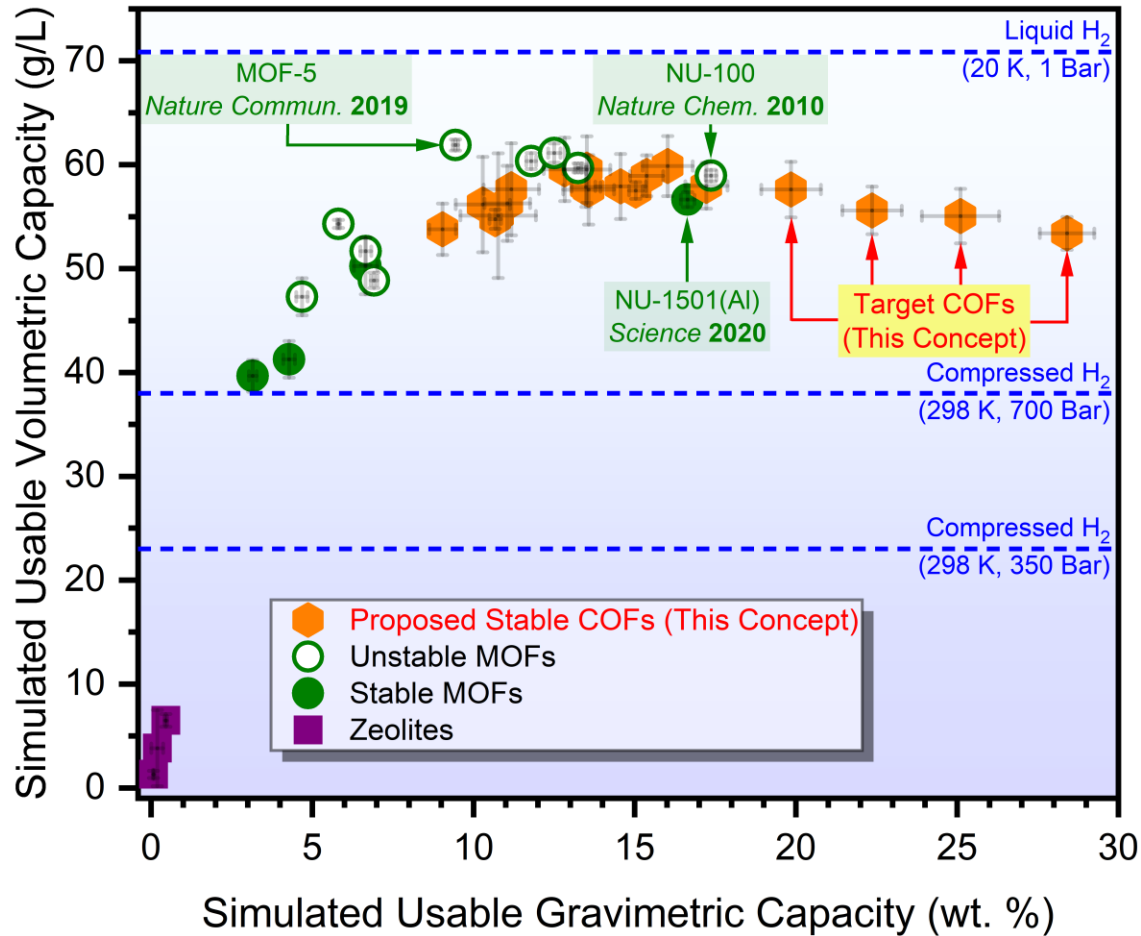
Vastly Underexplored Geometries

Building unit 1 \ Building unit 2	2-c Linear	3-c Triangle	4-c Square	4-c tet	6-c Hexagon	6-c oct
3-c Triangle	srs	bwt, pyo, srs-b, ths-b	fjh, fmj, gee, iab, yac, yao	asn, ept, ofp	cys, dnf*	anh, ant, apo, brk, cep*, cml, czz, eea, qom, rtl, tsx, zzz
4-c Square	nbo, lvt, rhr	pto, tbo	cev, cdl, cdm, cdu, cds, cdz, mot, muo, qdl, qzd, ssd, sse, ssf, sst	pts	nts	myd, ybh
4-c tet	dia, lcs, qtz, sod	bor, ctn	fgl, mog, pds, pth, pti, ptr, ptt	bnl, byl, cag, cbt, coe, crb, fel, icm, kea, lon, pcl, qtz-b, sca, tpd, ucn	-	alw, bix, cor, ing, spl, toc
6-c Hexagon	hxg	cys, dnf	she	-	hxg-b	-
6-c oct	pcu, bcs, crs, reo	pyr, spn	soc	gar, iac, ibd, toc	-	pcu-b, bcs-b
6-c trp	lcy, acs	ceq, dag, fmz, hwx, moo, sab, sit, ydq	stp	fsi, hea, tpt	htp	nia

Building unit 1 \ Building unit 2	2-c Linear	3-c Triangle	4-c Square	4-c tet	6-c Hexagon	6-c oct
8-c cub	bcu	the	scu, csq, sqc	flu	-	ocu
12-c cuo	fcu	sky	ftw	edc	-	-
12-c ico	-	-	-	ith	-	-
12-c hpr	-	aea	shp	-	-	-
12-c tte	-	ttt	-	-	mgc	-
24-c tro	-	-	-	twf	-	-

Computational Screening

H₂ Stores at 77 K, 100 Bar, Releases at 160 K, 5 Bar



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