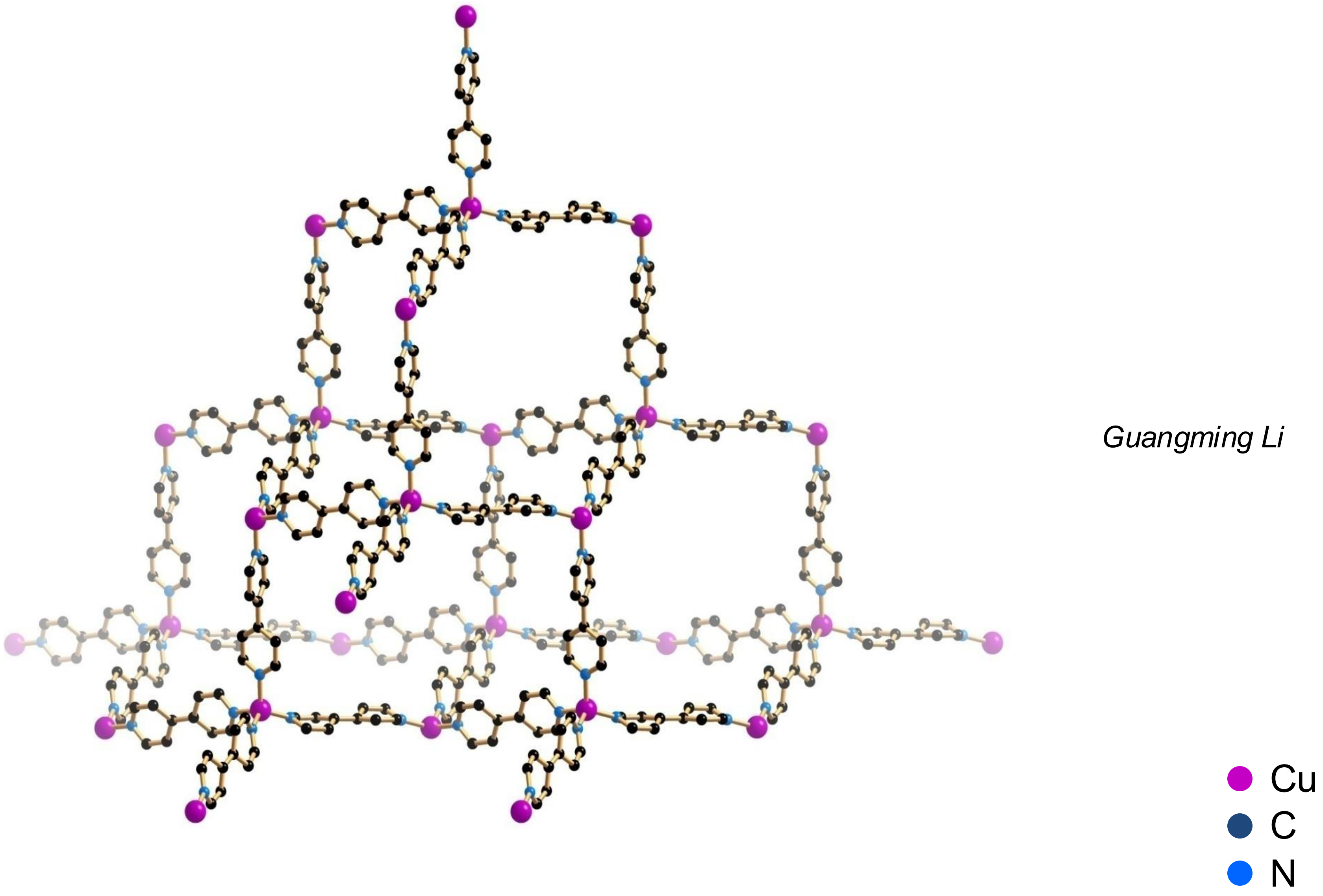
Nobel Lecture, Chemistry 2025

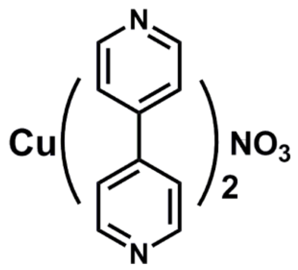
Metal-Organic Frameworks ↓ From Molecules to Society

Omar M. Yaghi
Department of Chemistry
Department of Materials Science and Engineering
Bakar Institute of Digital Materials for the Planet
University of California, Berkeley

Coordination Networks

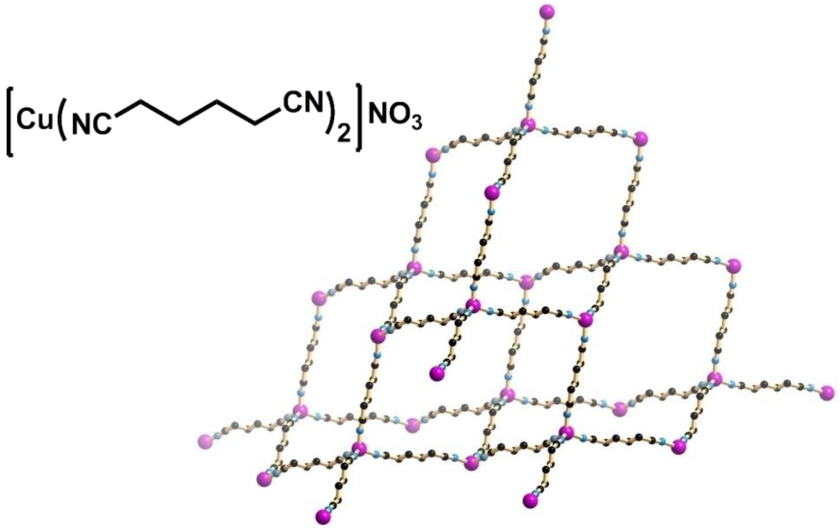


Guangming Li

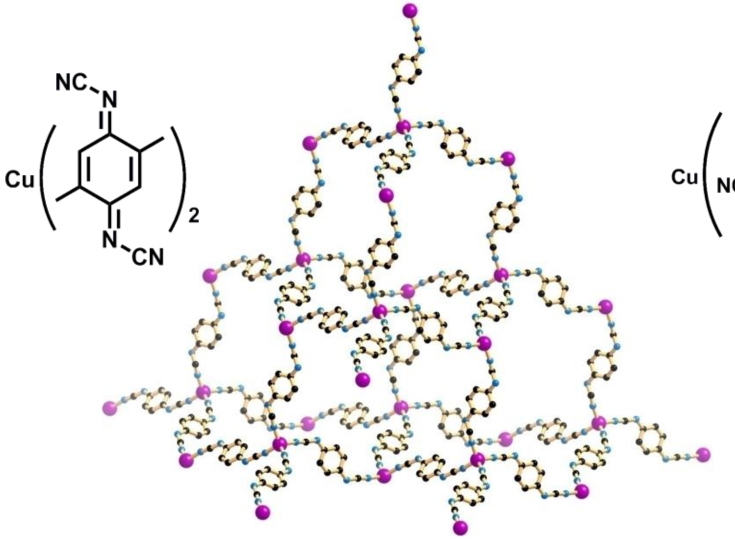


Yaghi, O. M., Richardson, D. A., Li, G., Davis, C. E., Groy, T. L. *Mater. Res. Soc. Symp. Proc.,* **1995**, 371, 15-19.

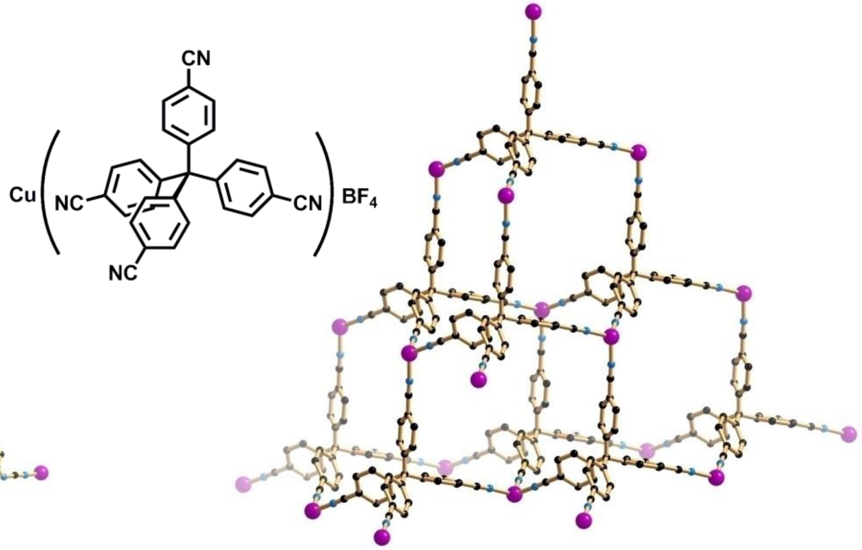
Early Coordination Networks



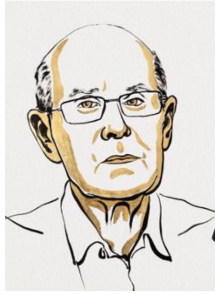
Y. Kinoshita, I. Matsubara and Y. Saito, *Bull. Chem. Soc. Jpn.*, **1959**, *32*, 741-747. Y. Kinoshita, I. Matsubara, T. Higuchi and Y. Saito, *Bull. Chem. Soc. Jpn.*, **1959**, *32*, 1221-1226. Y. Kinoshita, I. Matsubara and Y. Saito, *Bull. Chem. Soc. Jpn.*, **1959**, *32*, 1216-1221.



Aumüller, P. Erk, G. Klebe, S. Hünig, J. U. von Schütz and H.-P. Werner, *Angew. Chem., Int. Ed.*, **1986**, *25*, 740-741.



B. F. Hoskins and R. Robson, *J. Am. Chem. Soc.*, **1989**, *111*, 5962-5964.

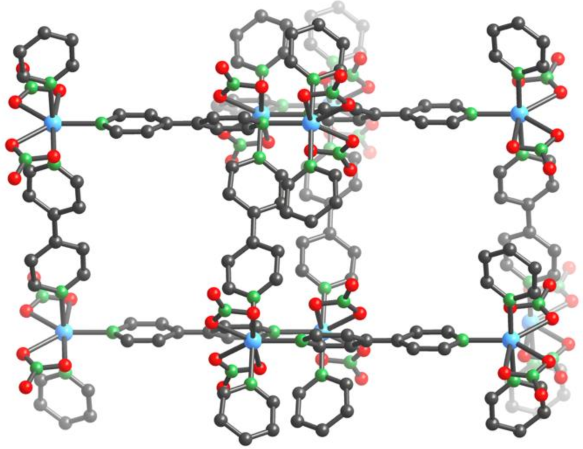


Richard Robson

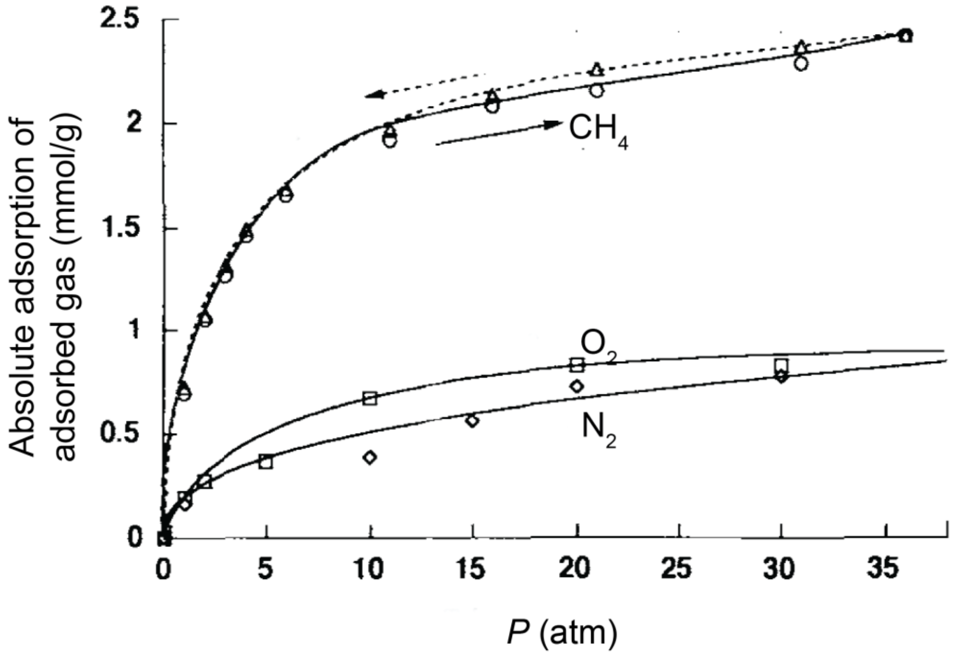
They were beautiful but frail...

Pressurized Gas Uptake by a Coordination Network

Susumu Kitagawa

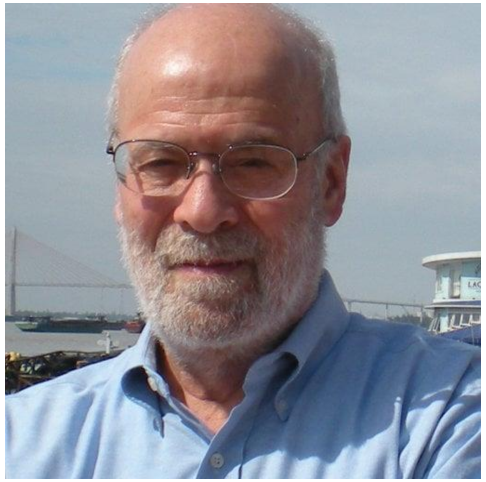


$\{[Co_2(4,4'\text{-bipyridine})_3(NO_3)_4]\cdot xH_2O\}_n$



M. Kondo, T. Yoshitomi, H. Matsuzaka, S. Kitagawa and K. Seki, *Angew. Chem., Int. Ed.*, **1997**, *36*, 1725-1727.

Science begins with doubt and questions…



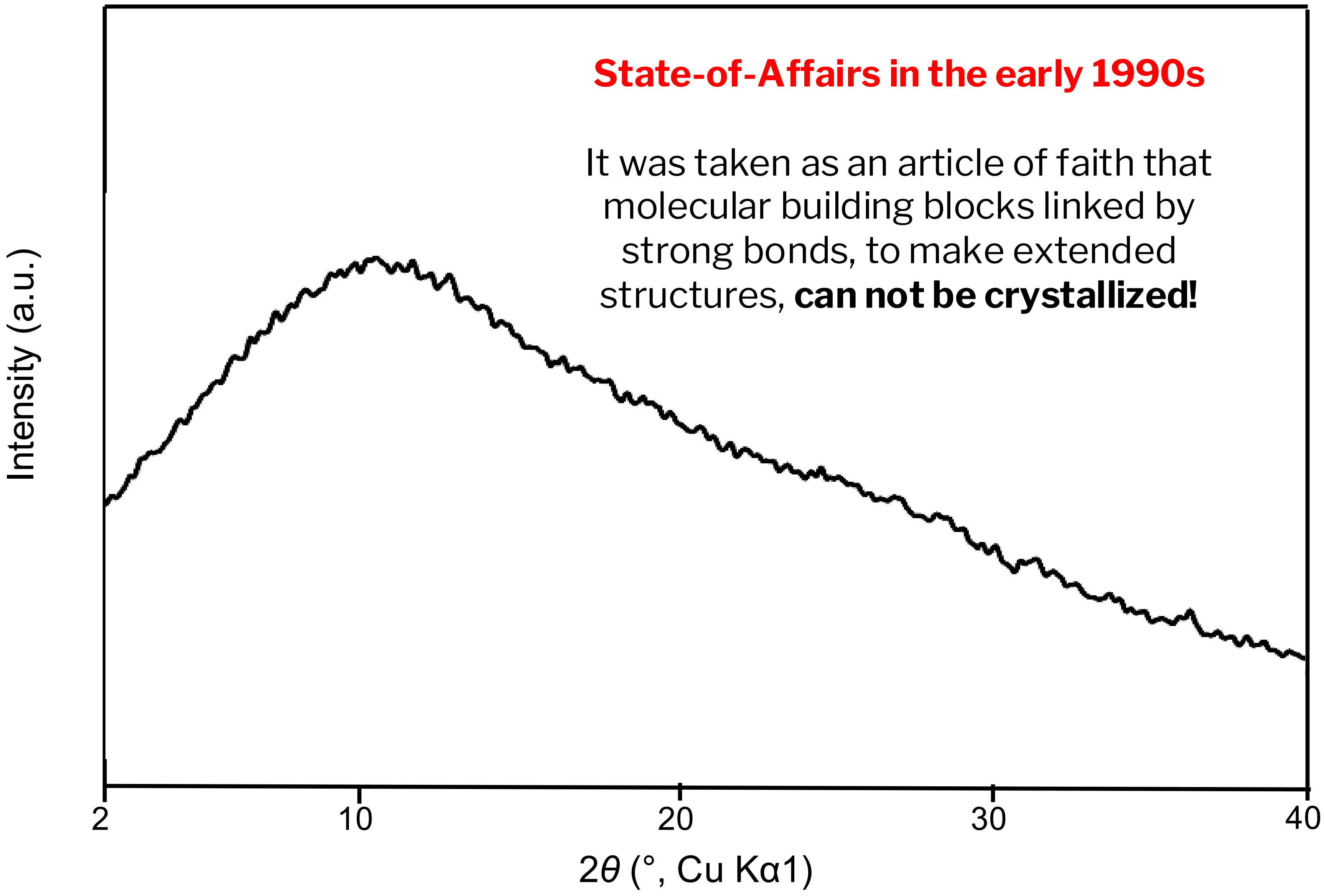
Walter Klemperer

Two important questions :

- Are the pores homogenous in size and shape?
- Do the pores remain open in the absence of any molecular guests?

We need to bond the constituent building blocks with strong bonds

Powder X-Ray Diffraction (PXRD) of a Poorly Crystalline/Amorphous Solid

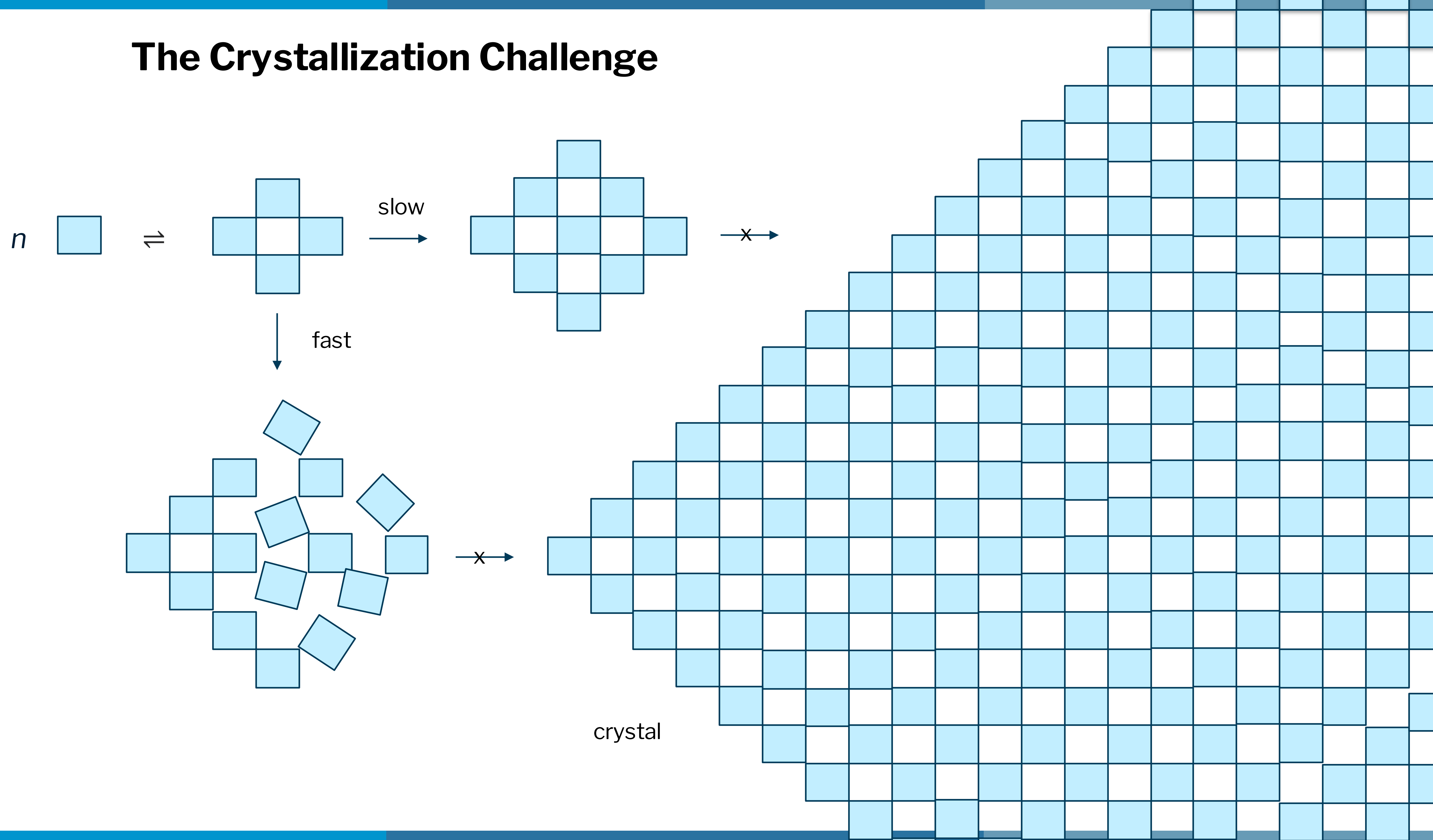


Science is an exercise in optimism…

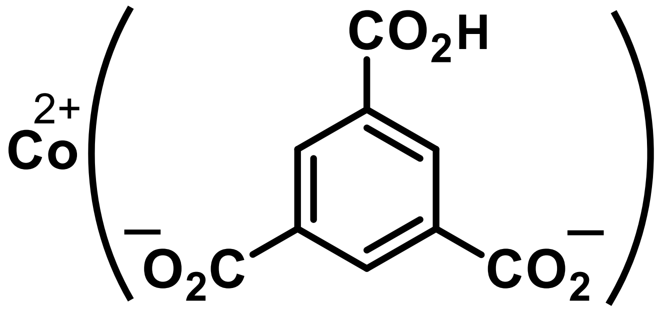
Richard Holm

O. M. Yaghi, This portrait of Marie Curie, *Molecular Frontiers Journal*, **2023**, 7, 1.

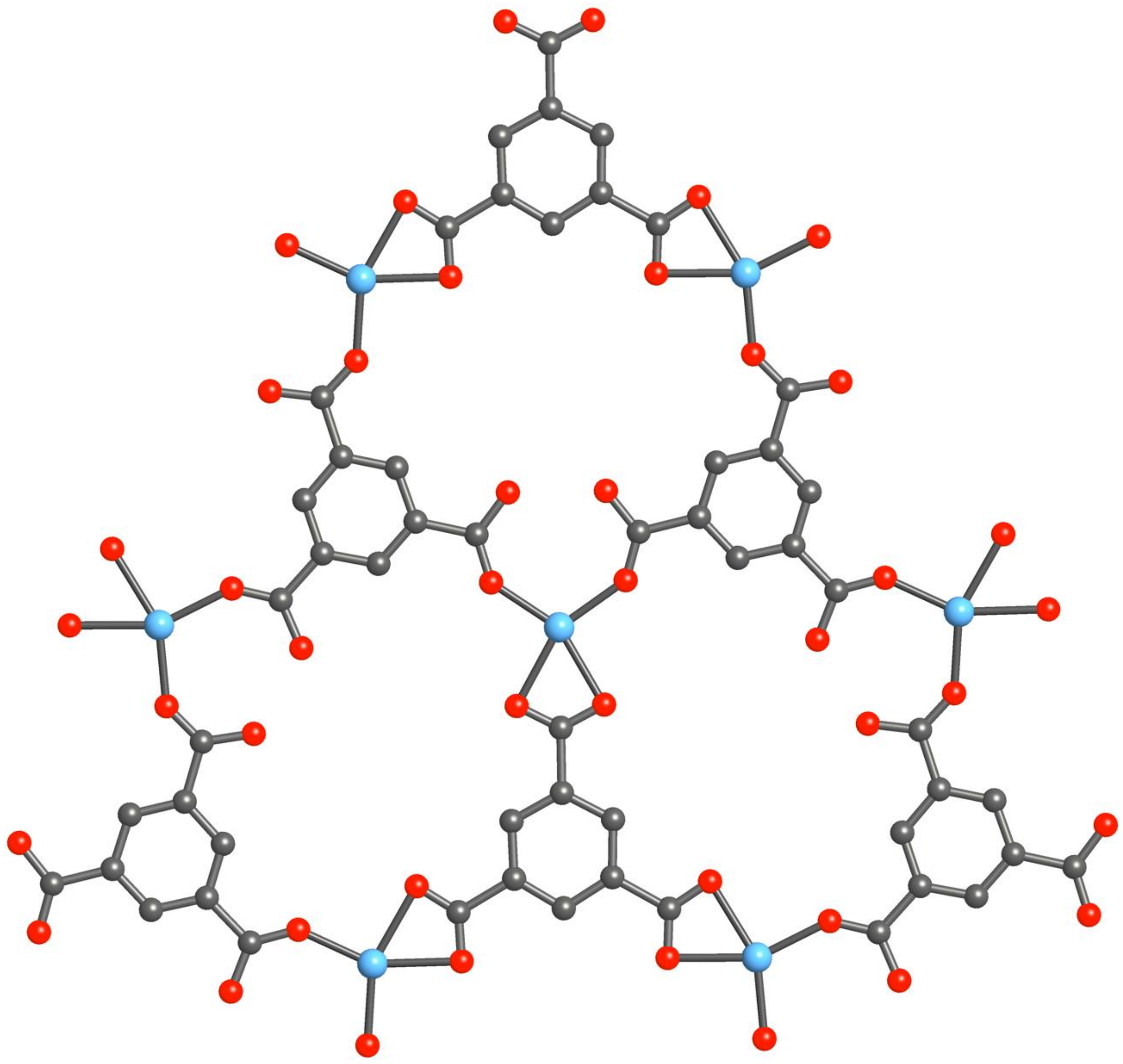
The Crystallization Challenge



First Crystallization of Metal-Organic Frameworks



Charged Linker



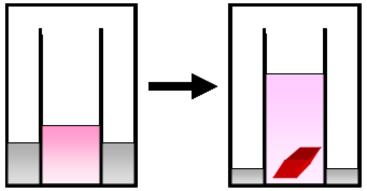
Guangming Li

O. M. Yaghi, G. Li and H. Li, *Nature,* **1995**, *378*, 703-706.

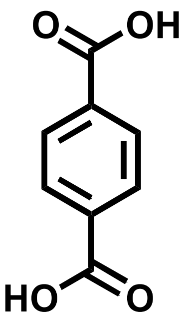
Metal-Organic Frameworks-2 (MOF-2)

Polynuclear metal oxide units, secondary building units (SBUs)

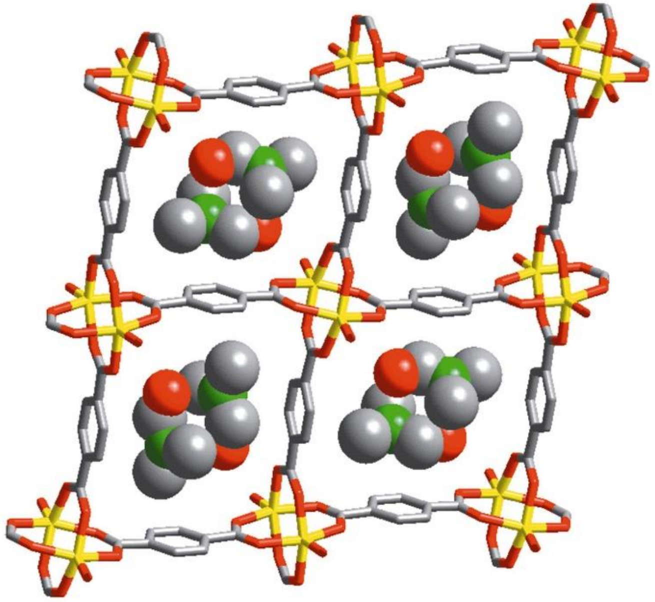
$$\underset{\substack{0.040\ \text{g}\\0.241\ \text{mmol}}}{H_2BDC} + \underset{\substack{0.073\ \text{g}\\0.246\ \text{mmol}}}{Zn(NO_3)_2{\bullet}4(H_2O)} \xrightarrow[\substack{(CH_3CH_2)_3N\\(0.05\ \text{ml}/5\ \text{ml Toluene})}]{\text{DMF}} Zn(BDC){\bullet}(DMF)(H_2O)$$



H_2BDC =



Benzenedicarboxylic acid

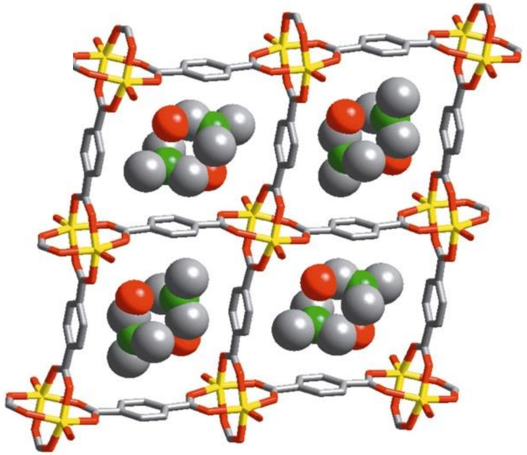


Hailian Li

H. Li, M. Eddaoudi, T. L. Groy and O. M. Yaghi, *J. Am. Chem. Soc.*, **1998**, *120*, 8571-8572.

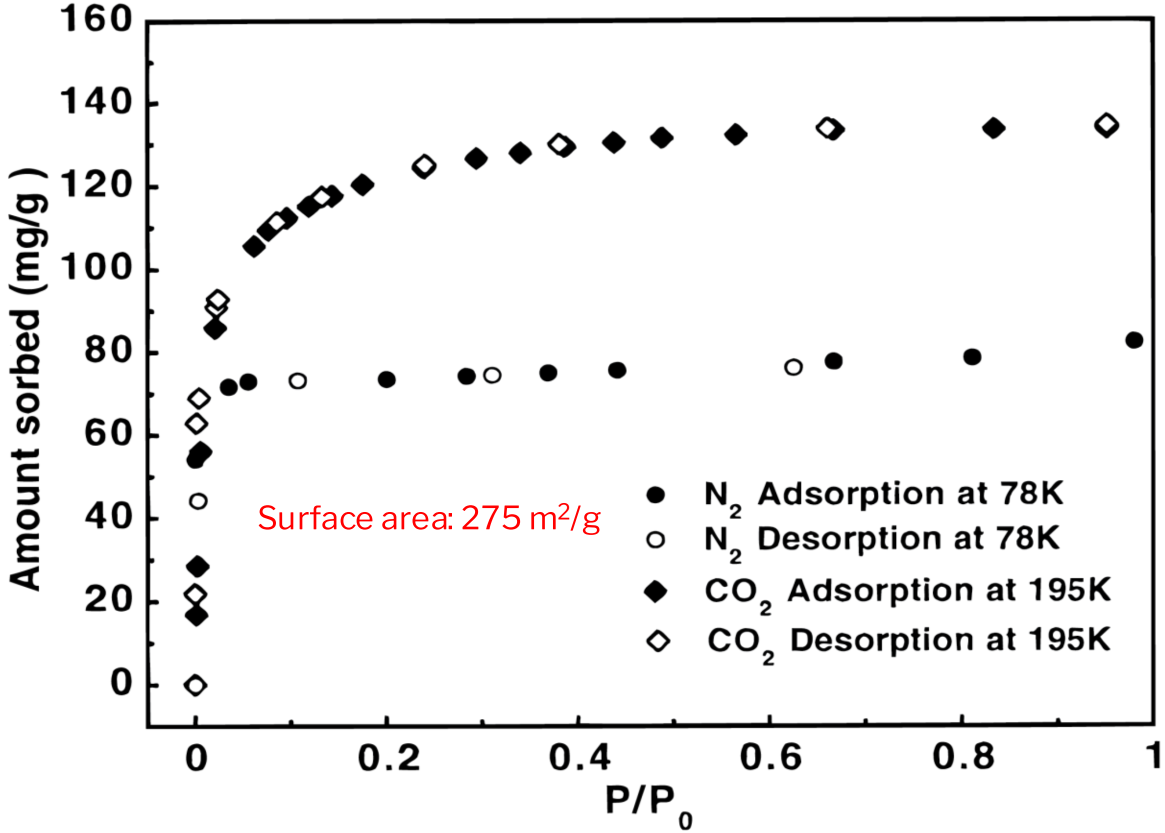
Gas adsorption isotherm of Metal-Organic Framework-2

Mohamed Eddaoudi



Zn(BDC)H_2O·DMF

Gas Adsorption Isotherm at 77 K:
Gold Standard for Determining
Permanent Microporosity



H. Li, M. Eddaoudi, T. L. Groy and O. M. Yaghi, *J. Am. Chem. Soc.*, **1998**, *120*, 8571-8572.

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MS NO: JA981669X-24-130-A

"This manuscript should be of wide appeal to a general audience interested in the synthesis and use of metal/organic porous materials. Invariably the porosities are generated by removal of solvents and organic groups or by topotactic structural rearrangement. Until now the major limitation of these materials has been in the ability to create systems with the necessary structural stability through low-temperature assembly techniques. This work is a benchmark for solving this problem."

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author; use additional blank pages if needed.)

JUN-17-98 WED 01:56 PM JACS PSU FAX NO. 814 8632855 P. 02

Review for JA981669X

LI ET AL.
ESTABISHING MICROPOROSITY IN OPEN METAL-
ORGANIC FRAMEWORKS:
GAS SORPTION ISOTHERMS

Reviewer B 6/15/98

This work represent a significant advance and demonstrates for the first time the microporosity which can be induced in the open framework metal-organics. The work is suitable for pulication in JACS. Some of the points below should be considered.

At least some of the diffraction data for the microporous material

"This work represent a significant advance and demonstrates for this first time the microporosity which can be induced in the open framework metal-organics."

understandable. Some speculation as to the nature of the partially activated compound would be welcome. p.4

Figure 2 is pretty but hardly described in the text. Sets of axes would help for both Figure 1 and 2.

I think the structure responsible for the sorption properties is NOT the structure reported. Figure 2 suggests the group has access to molecular modelling - and the text suggests a powder diffraction pattern (although broadened) is available. It really should not take much effort to index this pattern, take the building block in Figure 1 and move it about this cell to calculate a powder diffraction pattern. At least a reference to the data and what did not work should be given.

Review of Manuscript JA981669X-24-130-C by Li et al.

I agree with the authors when they state that the establishment of porosity in in the open metal-organic frameworks is important. This has been and continues to be a concern in publications involving this class of materials. In that regard, I find this paper refreshing. Below are listed several points that I would like to see addressed before publication (especially point 7).

p.4 last Paragraph

1. what is the particle size of the sample used for adsorption?

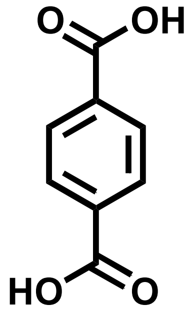
2. can the water and DMF be adsorbed to give the orginal material back?

3. are the nitrogen and carbon dioxide adsorptions reversible? what happens if carbon dioxide is adsorbed, desorbed and readsorbed? are the same

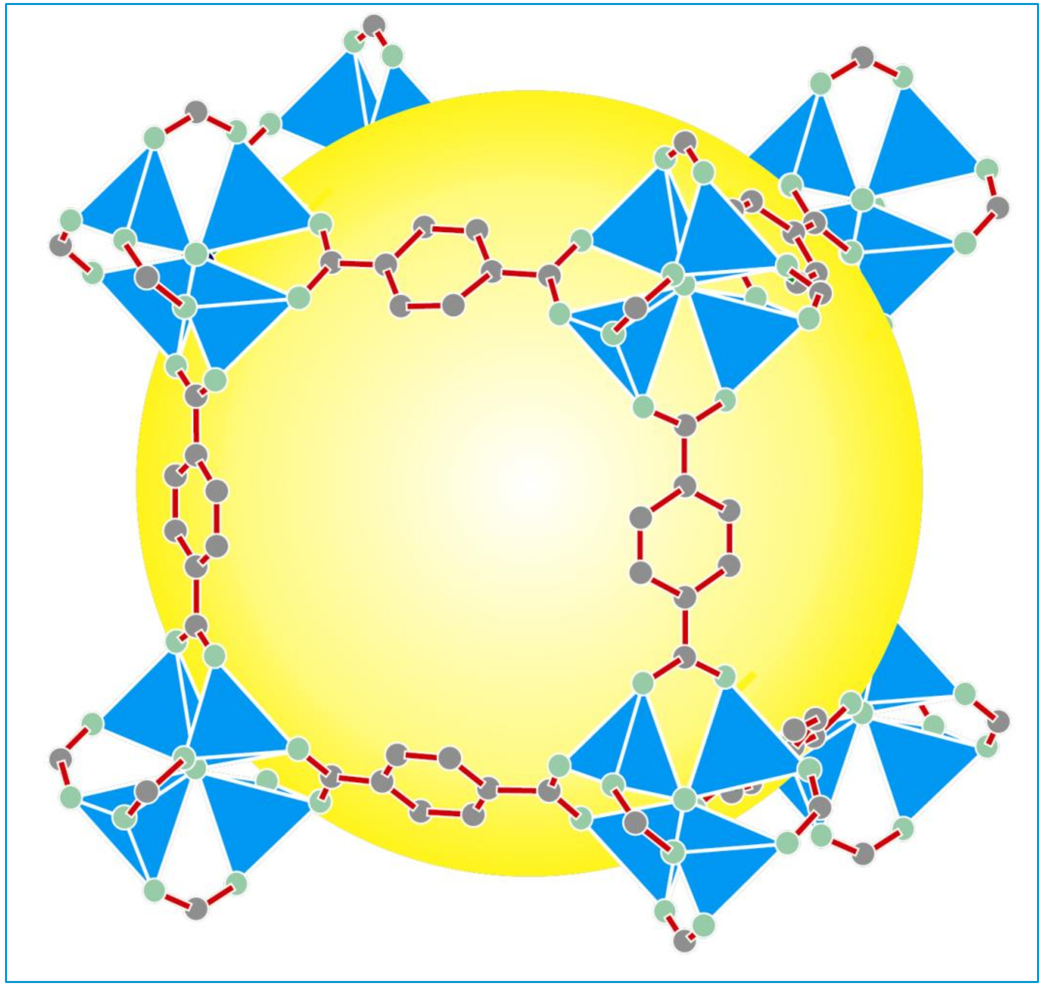
"I agree with the authors when they state that the establishment of porosity in the open metal-organic frameworks is important. This has been and continues to be a concern in publications involving this class of materials. In that regard, I find this paper refreshing."

Synthesis and crystal structure of MOF-5

$$H_2BDC + Zn(NO_3)_2{\bullet}4H_2O \xrightarrow[100\,^{\circ}C\,/\,20\,h]{DEF\,(12mL)} Zn_4O(BDC)_3{\bullet}(DEF)_7$$



H_2BDC



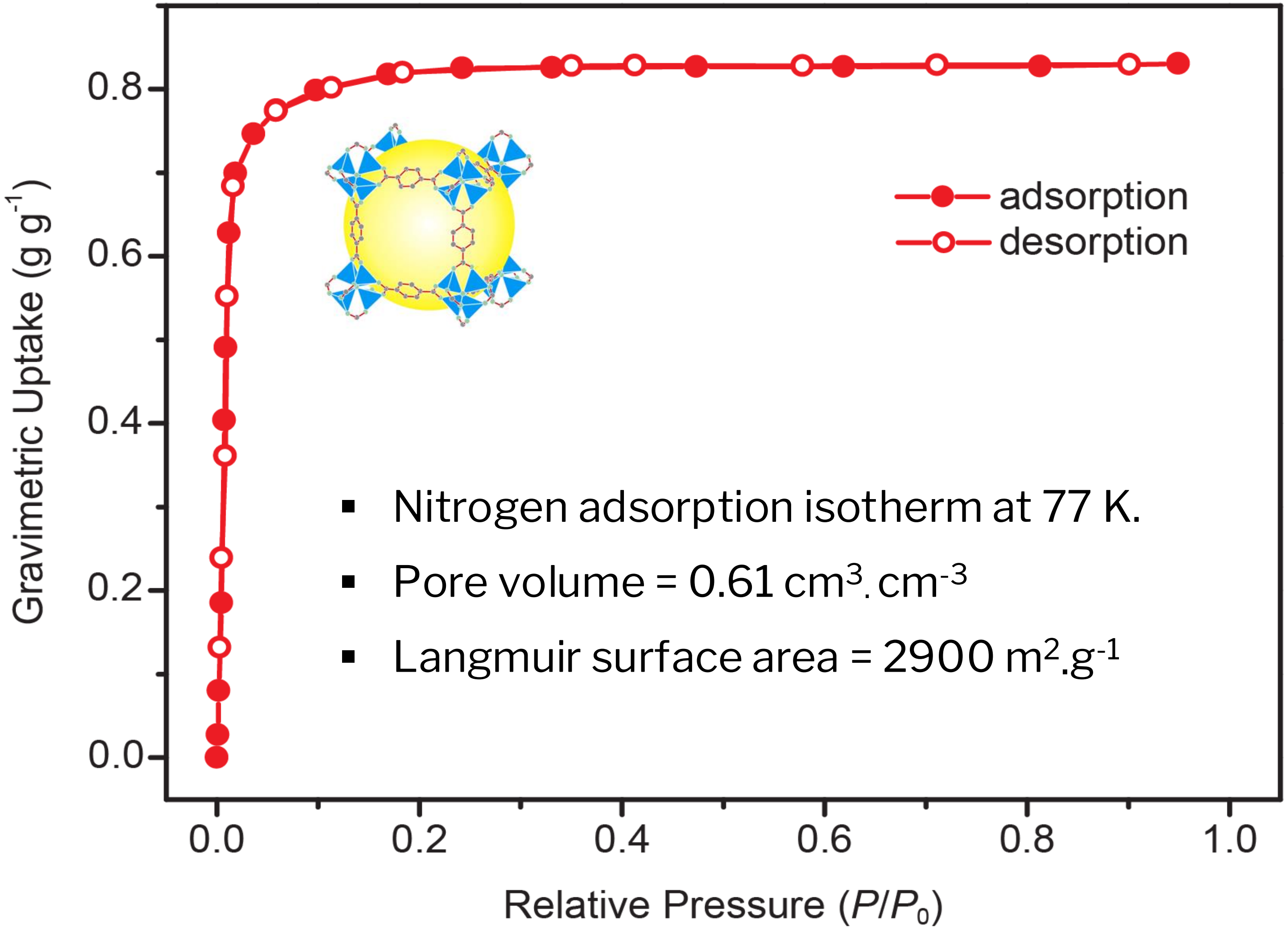
Cubic *Fm-3m*

a=25.6990(3) Å

V=16972.61 $Å^3$

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

Porosity of Metal-Organic Framework-5 (MOF-5)



- Nitrogen adsorption isotherm at 77 K.
- Pore volume = 0.61 $cm^3 . cm^{-3}$
- Langmuir surface area = 2900 $m^2 . g^{-1}$

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

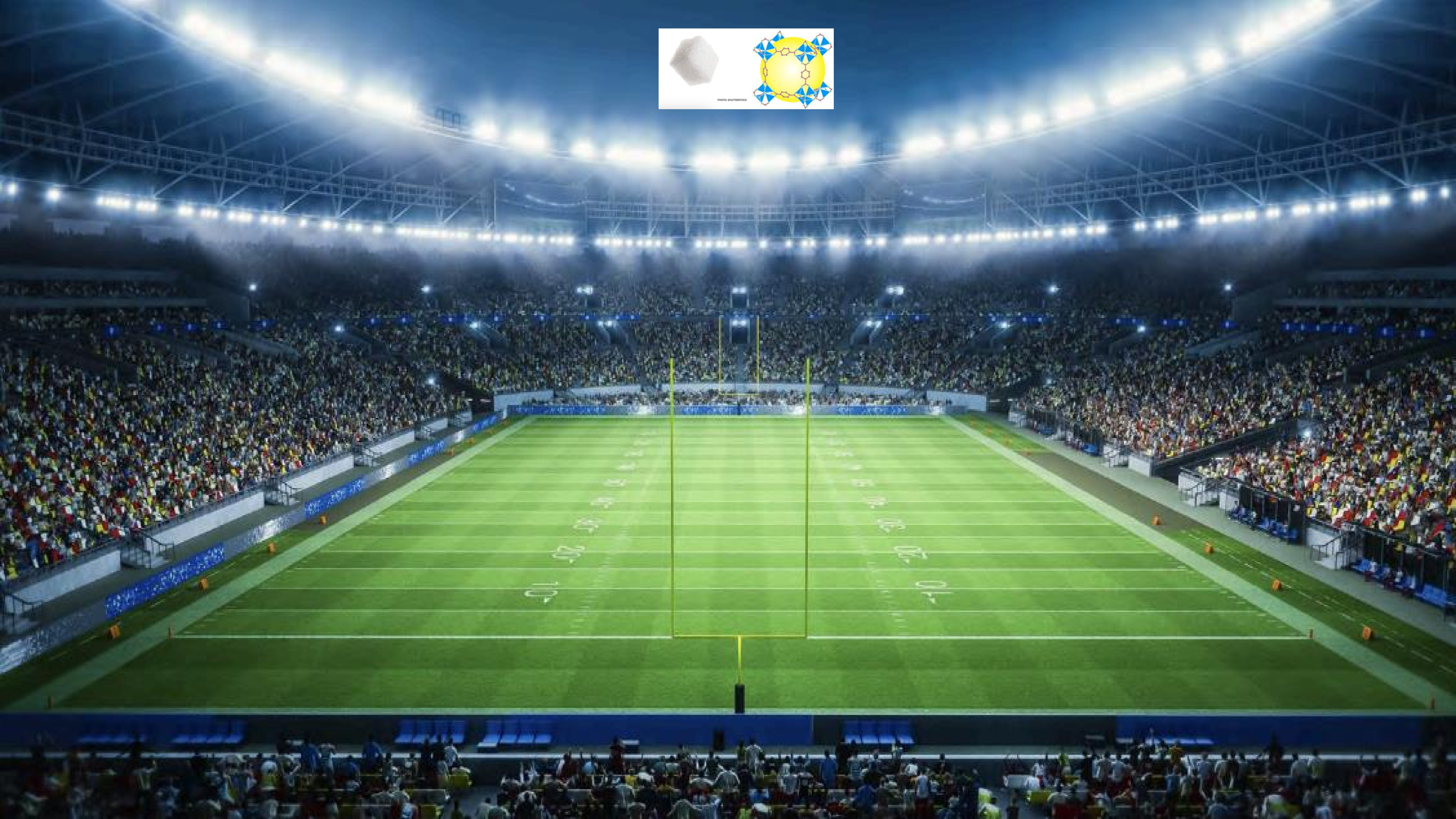
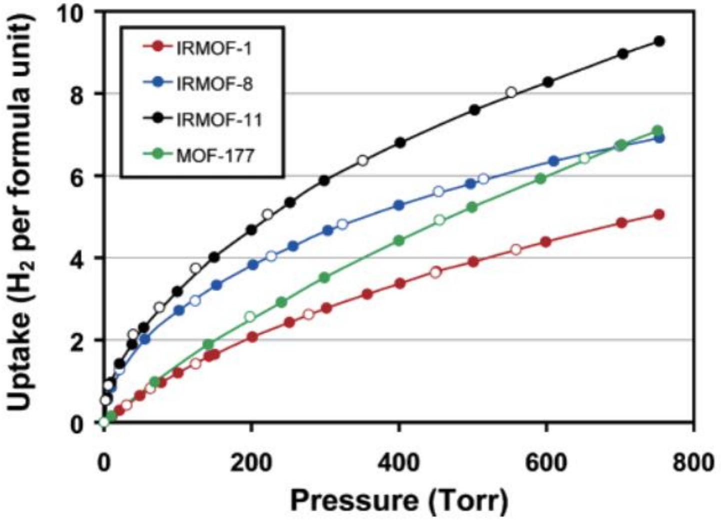


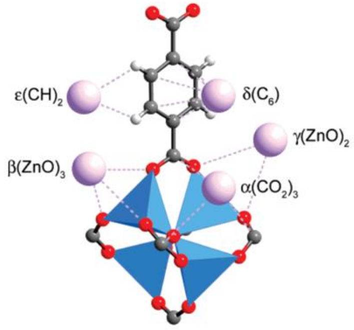
PHOTO: SHUTTERSTOCK


MOF-5 Crystals

Gas storage applications

H_2 Storage

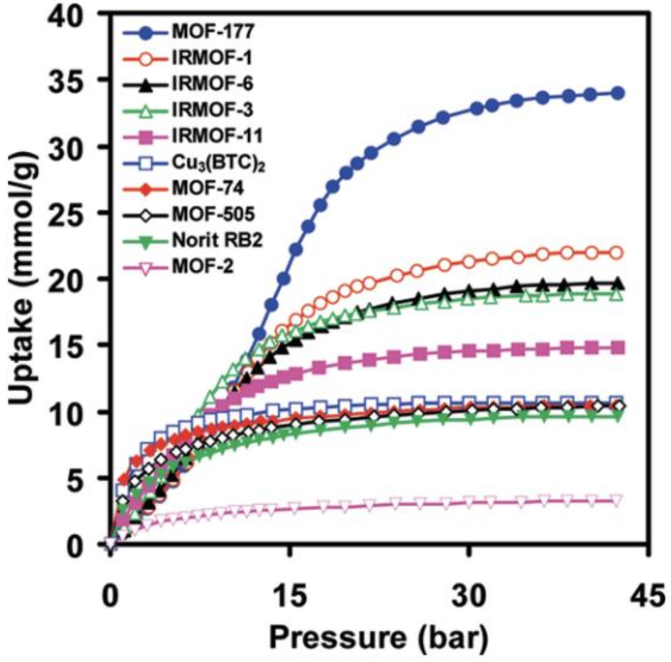


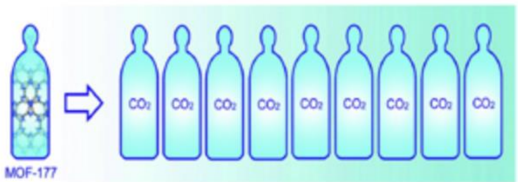


N. L. Rosi, M. Eddaoudi, D. T. Vodak, J. Eckert, M. O'Keeffe, O. M. Yaghi, *Science*, **2003**, *300*, 1127-1129.

J. L. C. Rowsell, A. R. Millward, K. S. Park, O. M. Yaghi, *J. Am. Chem. Soc.*, **2004**, *126*, 5666-5667.

CO_2 Storage

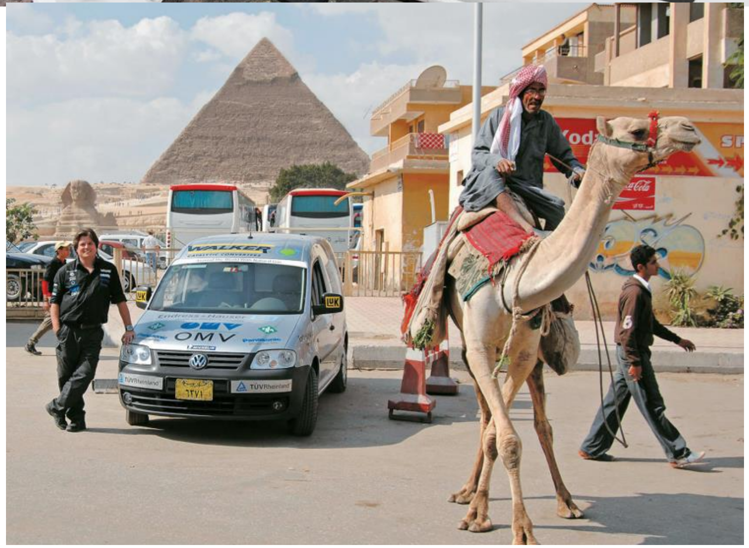




A. R. Millward, O. M. Yaghi, *J. Am. Chem. Soc.*, **2005**, *127*, 17998-17999.

D. Britt, H. Furukawa, B. Wang, T. G. Glover, O. M. Yaghi, *Proc. Natl. Acad. Sci. U.S.A.*, **2009**, 106, 20637-20640.

CH_4 Storage



Metal-Organic Frameworks with High Capacity and Selectivity for Toxic Gases

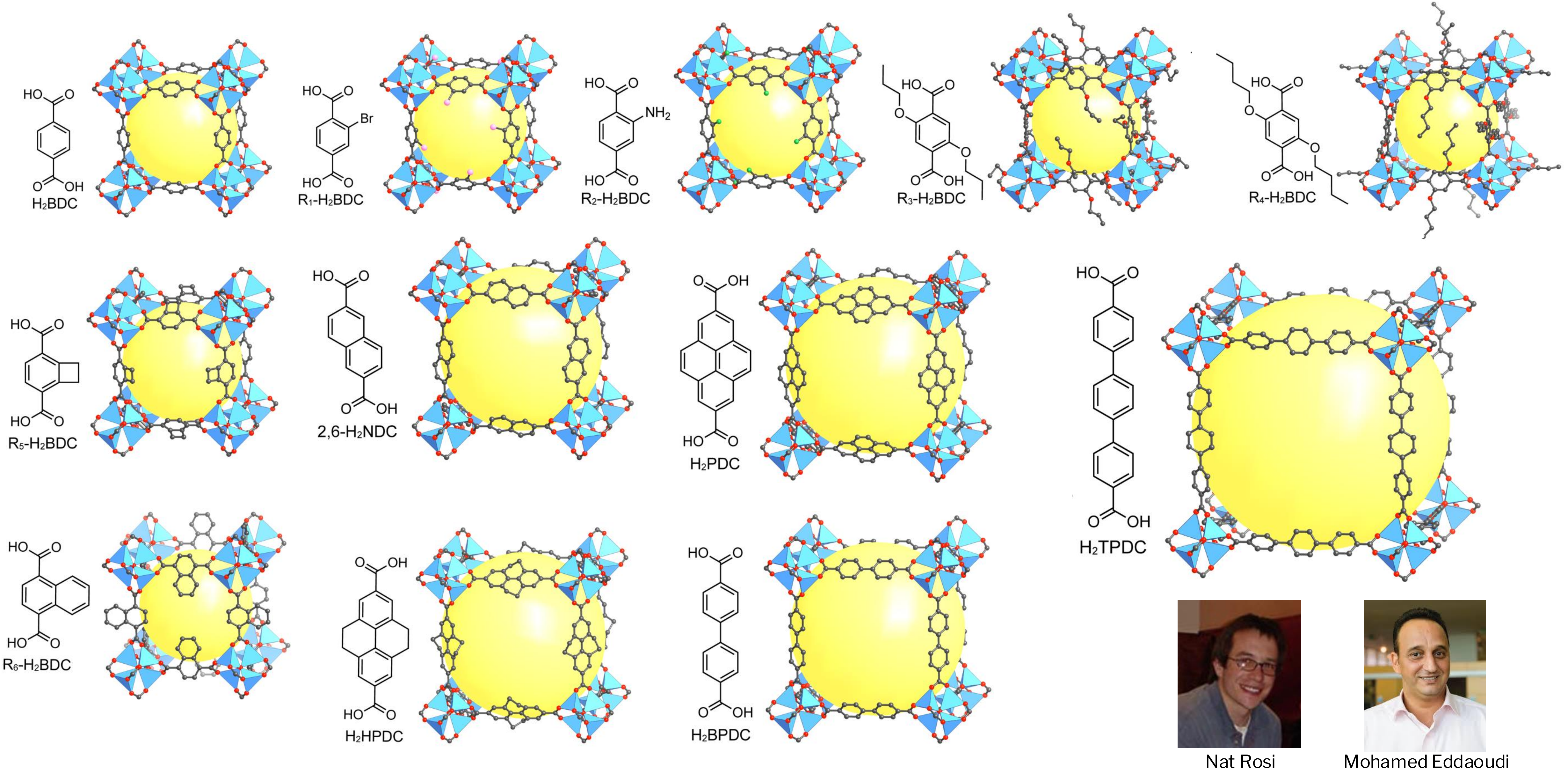
Table 2. Dynamic adsorption capacities of the benchmark MOFs for gaseous contaminants measured in grams of gas per gram of adsorbent

Gas	MOF-5	IRMOF-3	MOF-74	MOF-177	MOF-199	IRMOF-62	BPL carbon	Improvement factor*
Sulfur dioxide	0.001	0.006	0.194†	<0.001	0.032	<0.001	0.033	5.88
Ammonia	0.006	0.105†	0.093	0.042	0.087	0.023	0.001	105
Chlorine	‡	0.335†	‡	<0.001	0.036	0.092	0.190	1.76
Tetrahydrothiophene	0.001	0.007	0.090	<0.001	0.351†	0.084	0.123	2.85
Benzene	0.002	0.056	0.096	0.001	0.176†	0.109	0.155	1.14
Dichloromethane	<0.001	0.001	0.032	<0.001	0.055†	0.019	0.053	1.04
Ethylene oxide	0.001	0.002	0.110	<0.001	0.095†	0.011	0.010	9.50

*Expresses the ratio of dynamic adsorption capacity of the best-performing MOF (†) to that of BPL carbon.
†Best-performing MOFs.
‡Experiments were not performed because of corrosion of the apparatus by chlorine.

D. Britt, D. J. Tranchemontagne, O. M. Yaghi, *Proc. Natl. Acad. Sci. U.S.A.*, **2008**, *105*, 11623-11627.

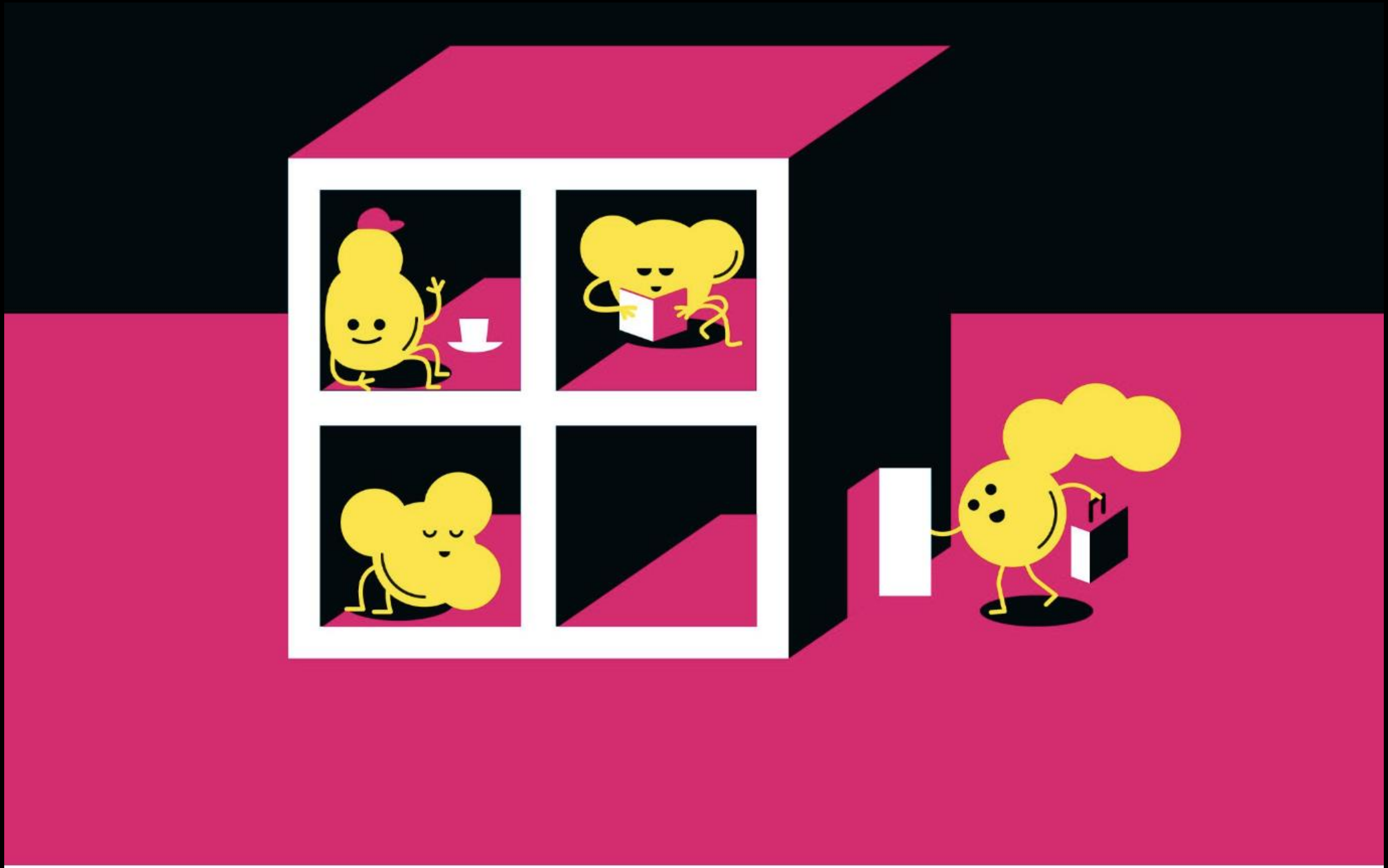
Isoreticular Metal-Organic Frameworks



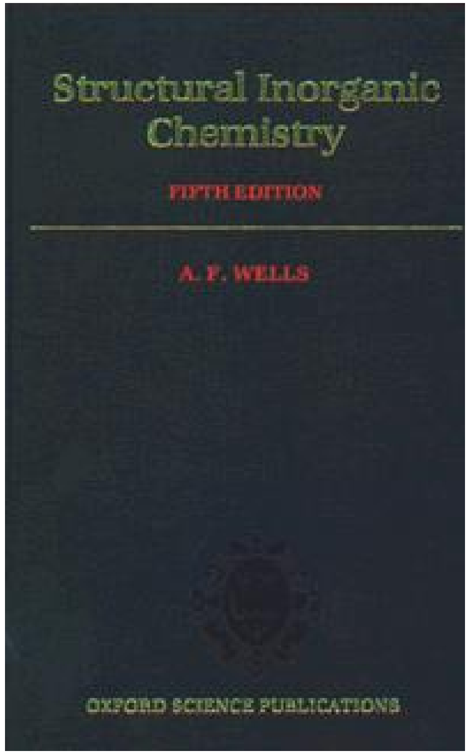
M. Eddaoudi, J. Kim, N. Rosi, D. Vodak, J. Wachter, M. O'Keeffe and O. M. Yaghi, *Science*, **2002**, *295*, 469-472.

"Rooms for Chemistry"

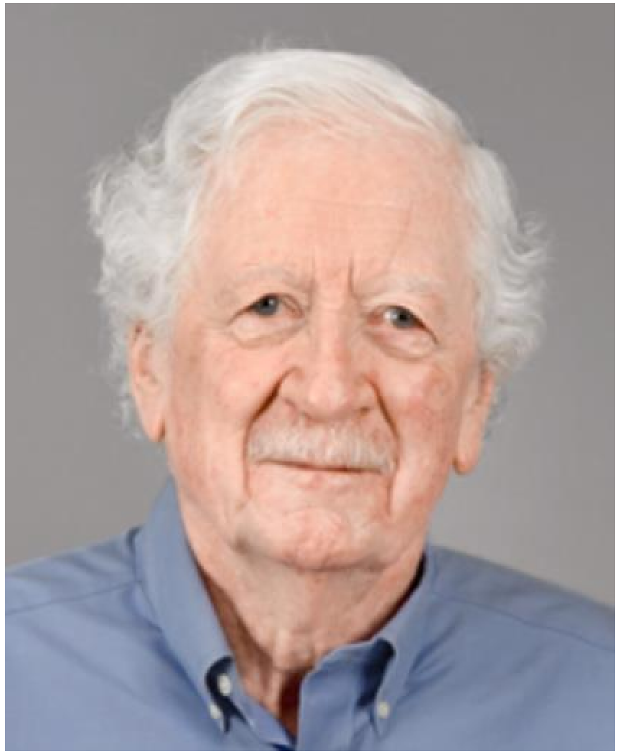
—Nobel Prize Chemistry Committee



The Idea of Nodes and Links Extended to MOFs



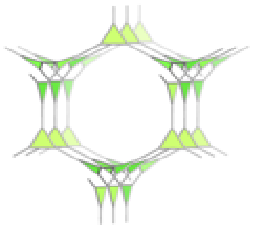
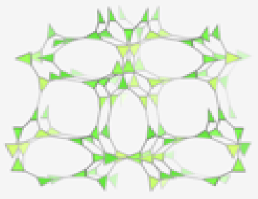
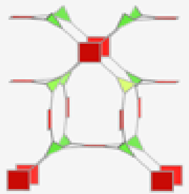
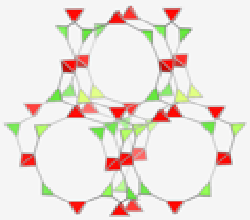
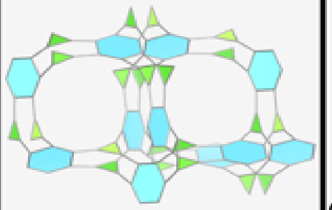
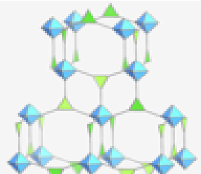
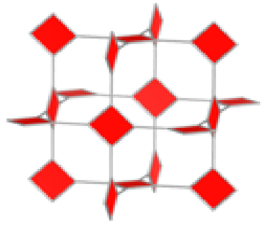
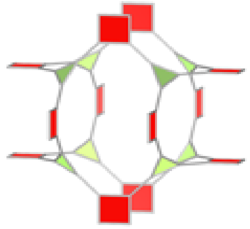
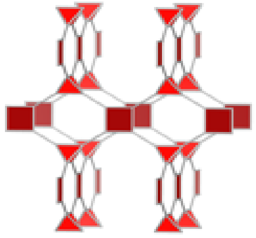
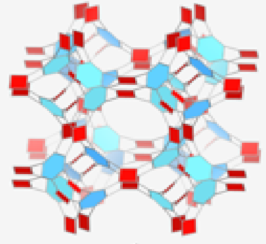
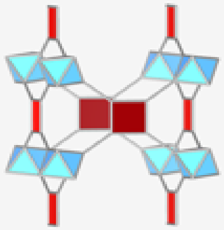
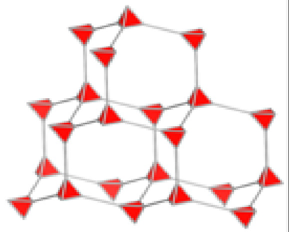
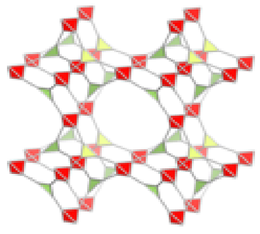
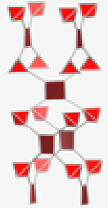
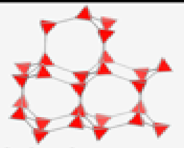
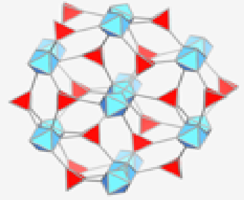
A. F. Wells, 1st to 5th Editions
1945 to 1984

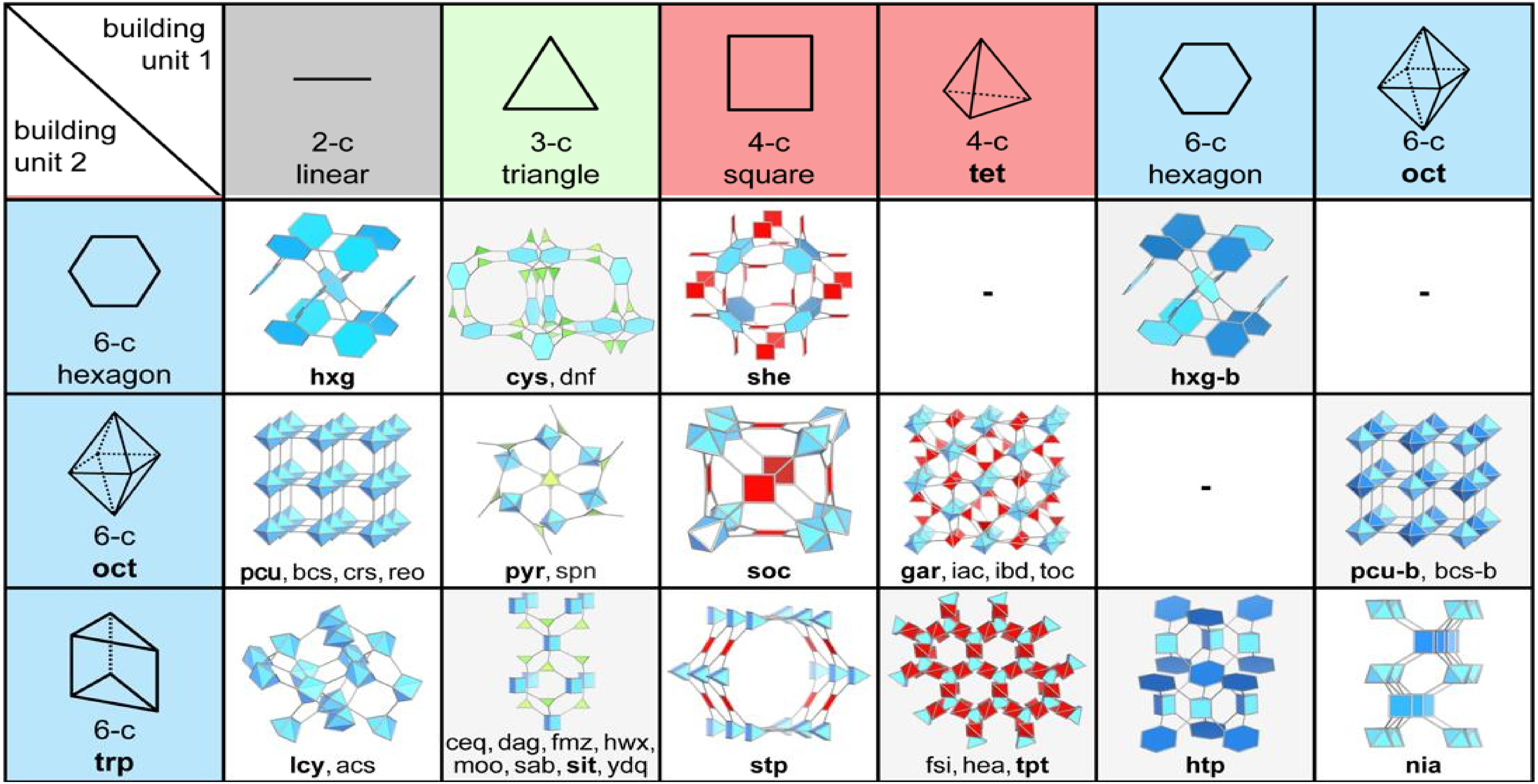


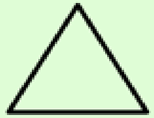
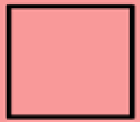
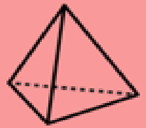
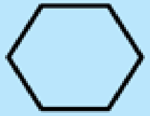
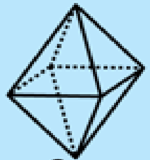
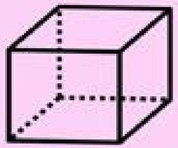
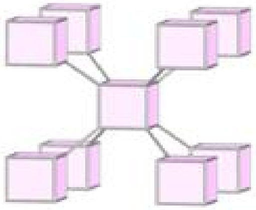
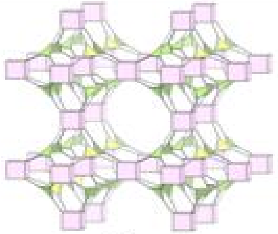
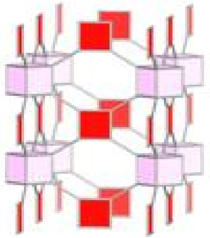
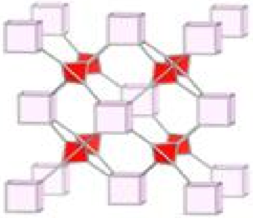
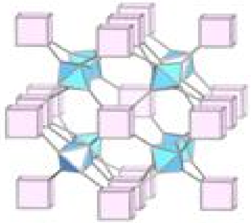
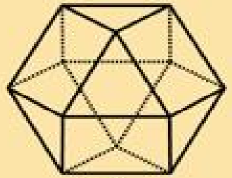
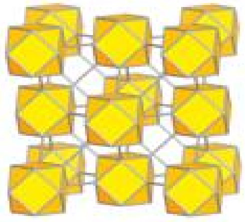
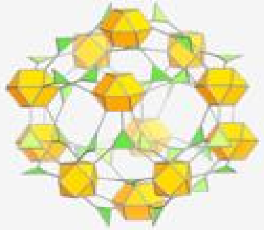
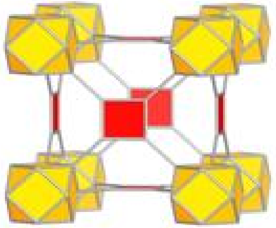
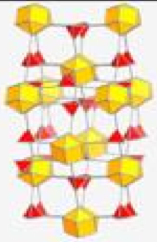
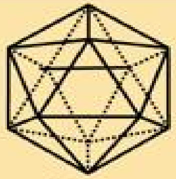
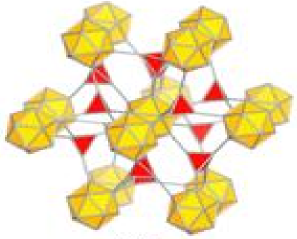
Michael O'Keeffe
Arizona State University

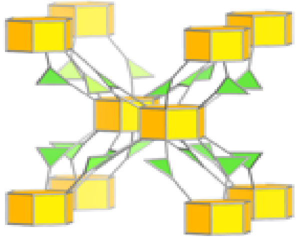
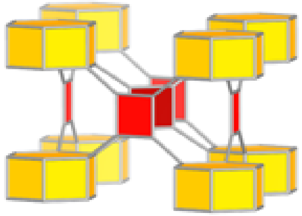
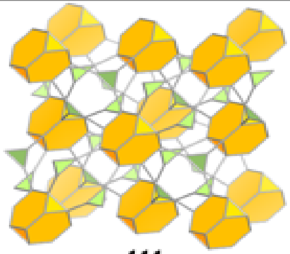
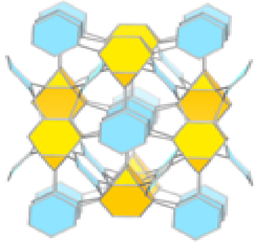
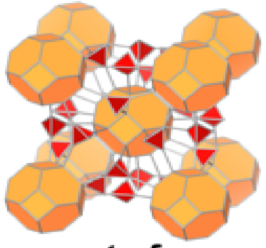
Davide Proserpio
University of Milan, Italy

The ‘Periodic’ Table of MOF Chemistry

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, cdn, 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


building unit 1
building unit 2
2-c linear
3-c triangle
4-c square
4-c tet
6-c hexagon
6-c oct
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**	-	-

building unit 2 \ building unit 1	2-c linear	3-c triangle	4-c square	4-c **tet**	6-c hexagon	6-c **oct**
12-c **hpr**	-	 **aea**	 **shp**	-	-	-
12-c **tte**	-	 **ttt**	-	-	 **mgc**	-
24-c **tro**	-	-	-	 **twf**	-	

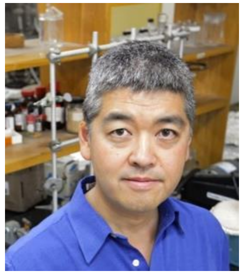
Dr. Markus Kalmutzki

M. Kalmutzki, N. Hanikel, O. M. Yaghi, *Sci. Adv.* **2018**, *4*, eaat9180.


Ulrich Müller

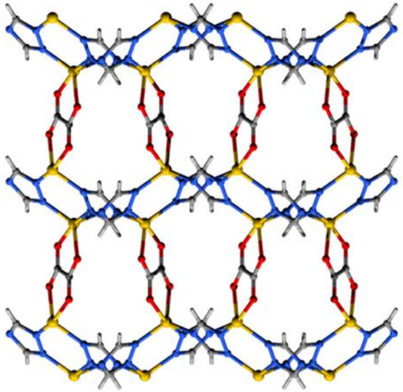
Tonne Scale-Up of MOFs

MOF systems for CO_2 Capture from cement plants in Canada

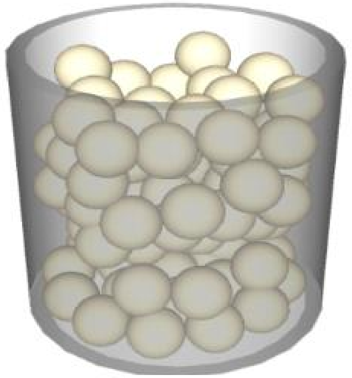


George Shimizu
Prof. of Chemistry
University of Calgary

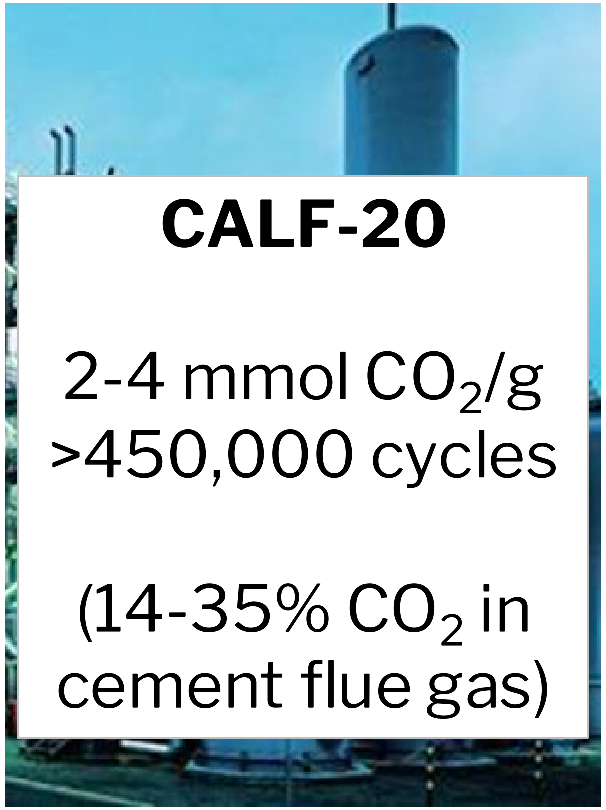
MOF
Crystal / Powder

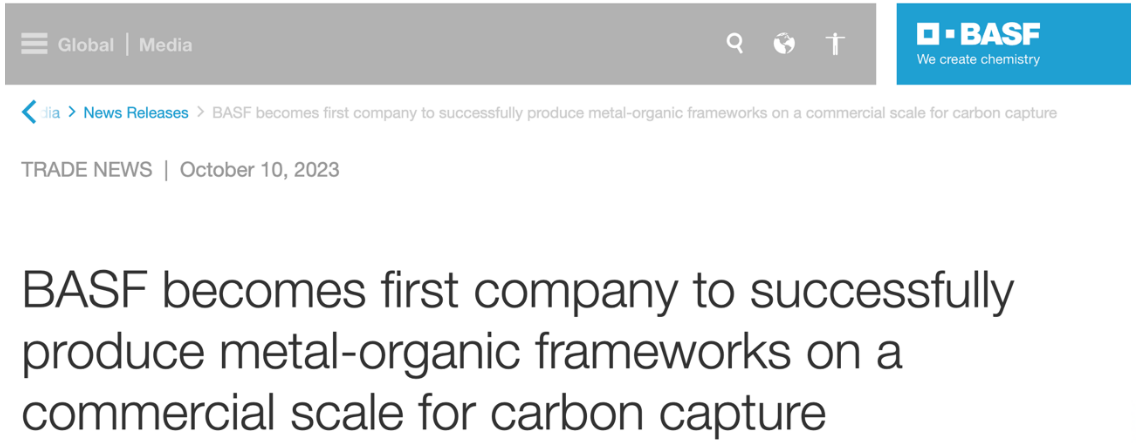


Structured
Powder



Engineering
Infrastructure
(PSA, TSA, VSA, etc.)





Global | Media

BASF
We create chemistry

dia > News Releases > BASF becomes first company to successfully produce metal-organic frameworks on a commercial scale for carbon capture

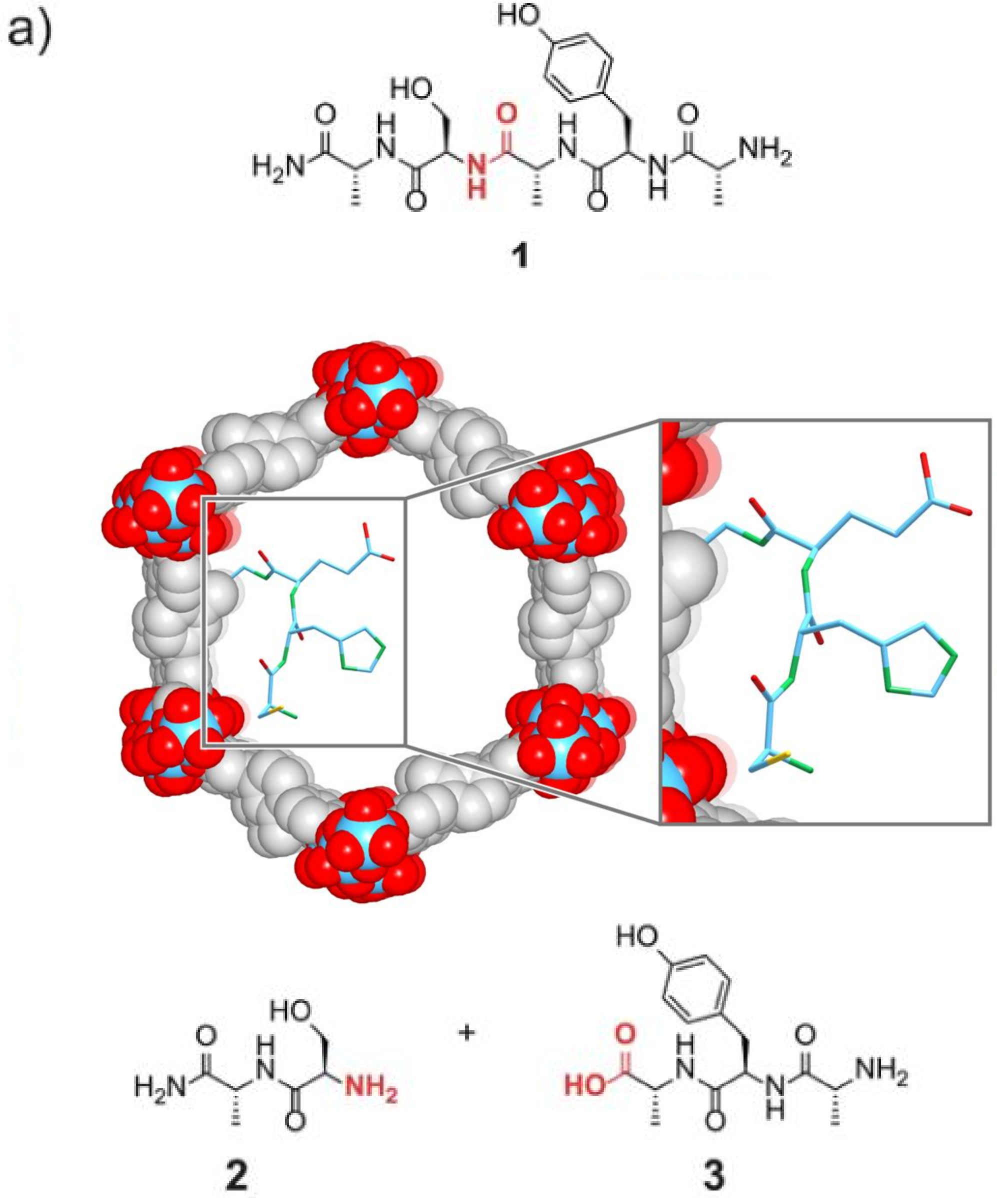
TRADE NEWS | October 10, 2023

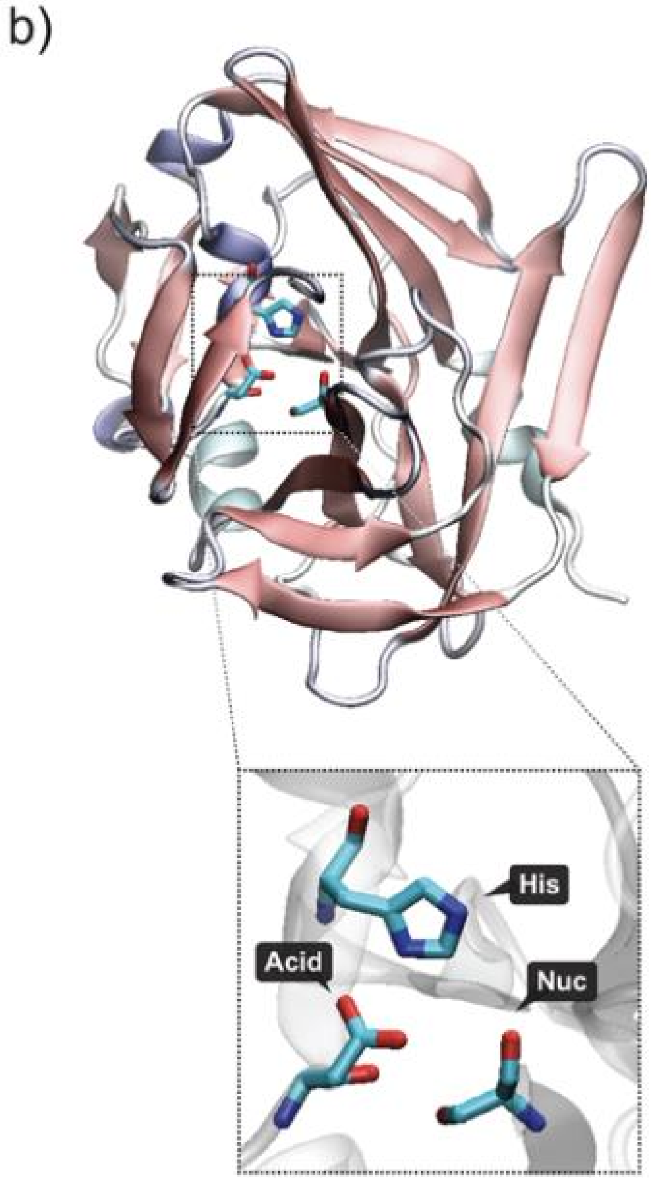
BASF becomes first company to successfully produce metal-organic frameworks on a commercial scale for carbon capture

What about the future?

Enzyme-like Complexity and Reactivity Within Multivariate MOFs

Alejandro Fracaroli





Enzyme **TEV protease** contains a catalytic triad of amino acids (red) that binds the substrates (black) in specific positions

Fracaroli, A.; Siman, P.; Nagib, D.; Suzuki, M.; Furukawa, H.; Toste, F. D.; Yaghi, O. M. *J. Am. Chem. Soc.*, **2016**, *138*, 8352-8355.

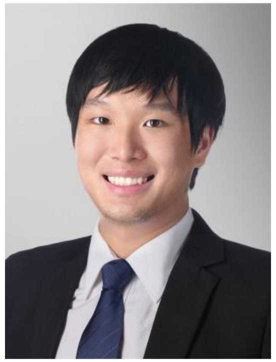
Aimatry

AIMATRY

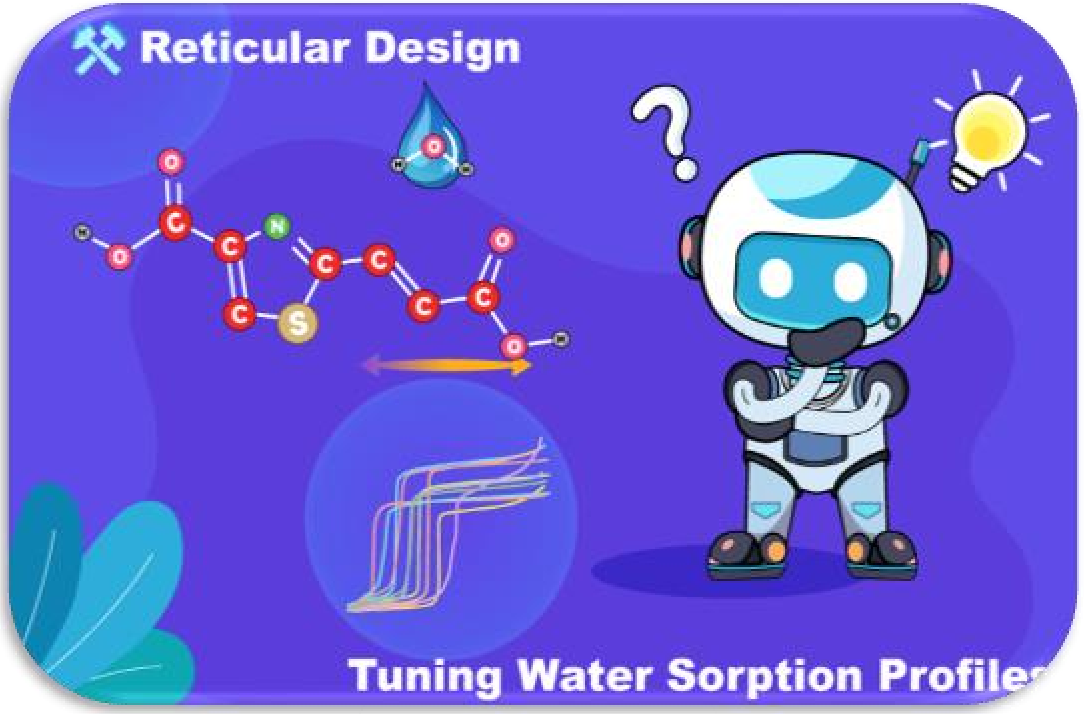
AI × MAterials × chemisTRY

The science of using AI for the design and synthesis of materials and for connecting chemical structures to properties and *vice versa*

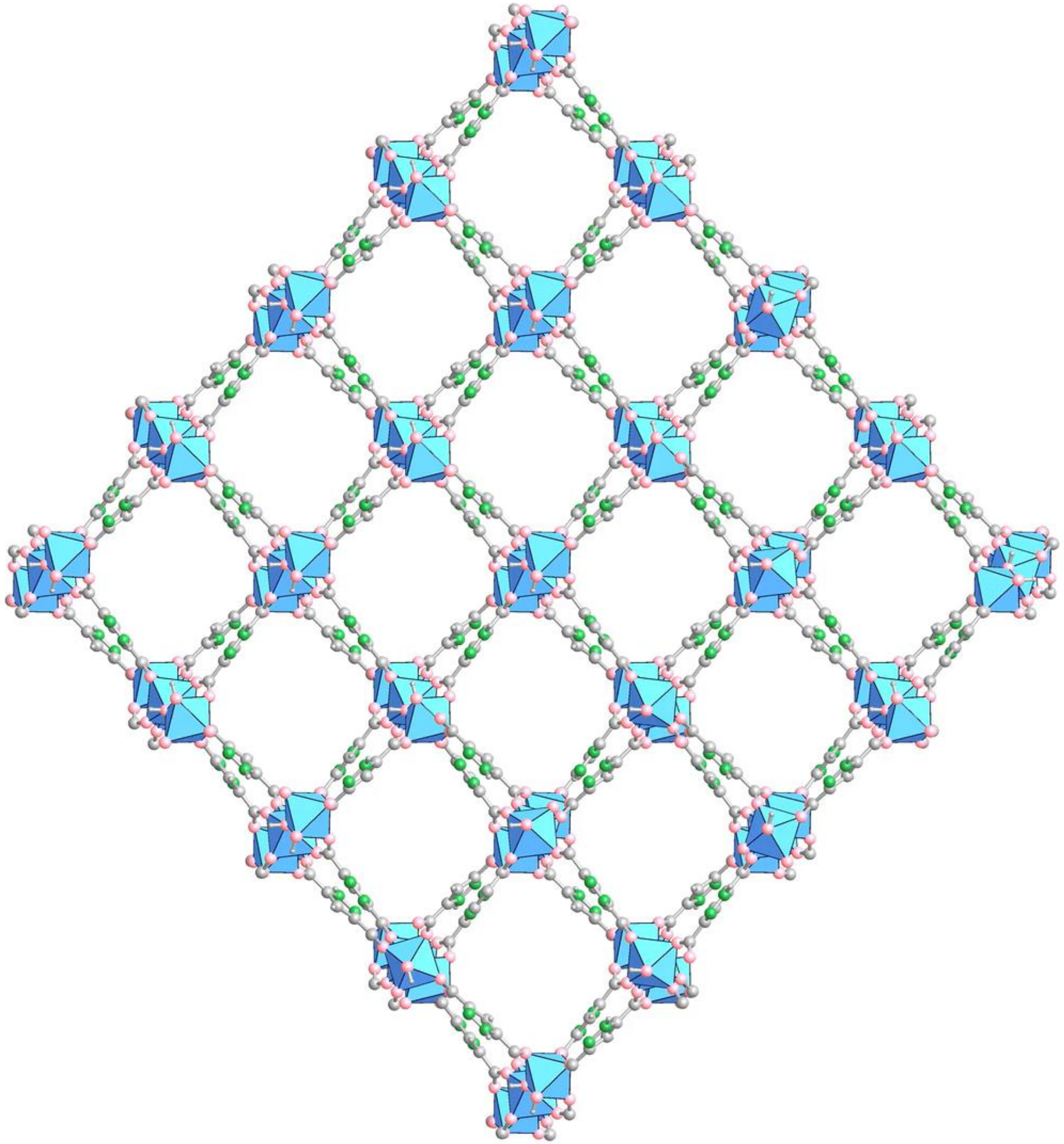
Molecular Editing by ChatGPT to improve water harvesting properties



Zach Zheng

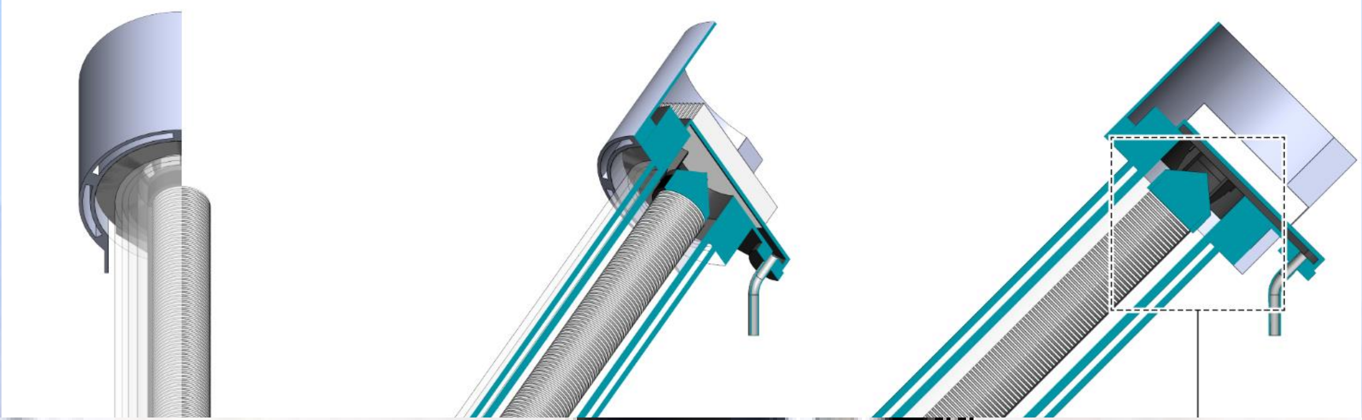


Mechanism of Water Harvesting in MOFs



Nikita Hanikel

N. Hanikel, X. Pei, S. Chheda, H. Lyu, W. Jeong, J. Sauer, L. Gagliardi, O. M. Yaghi, *Science*, **2021**, *374*, 454-459.



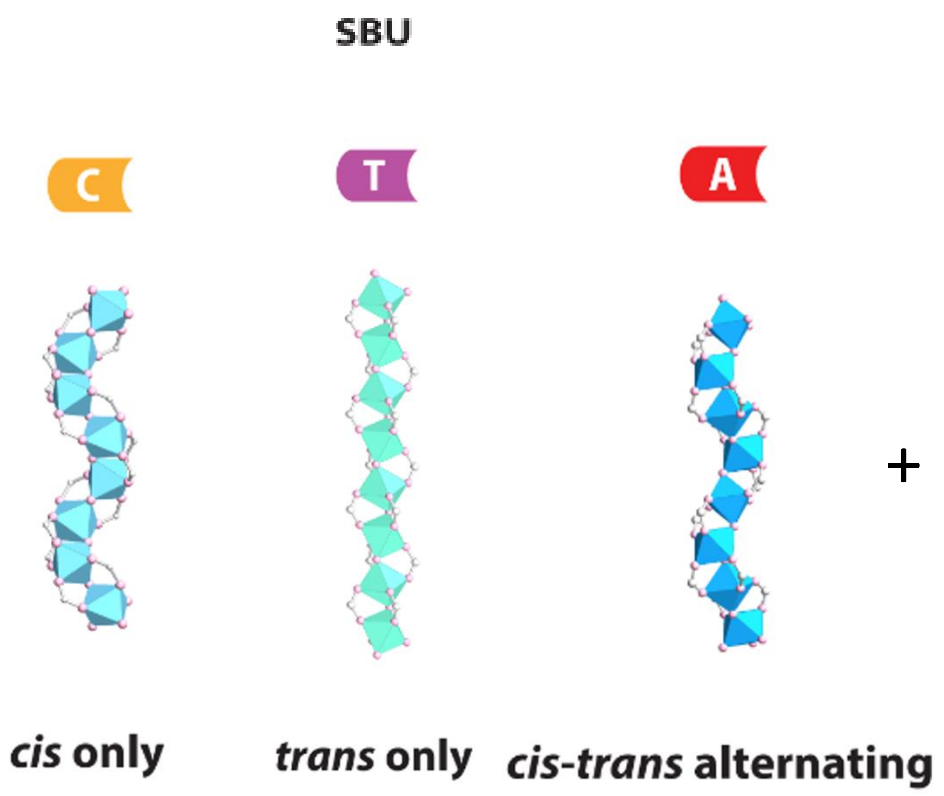
Ali Alawadi, Woochul Song, and Zac

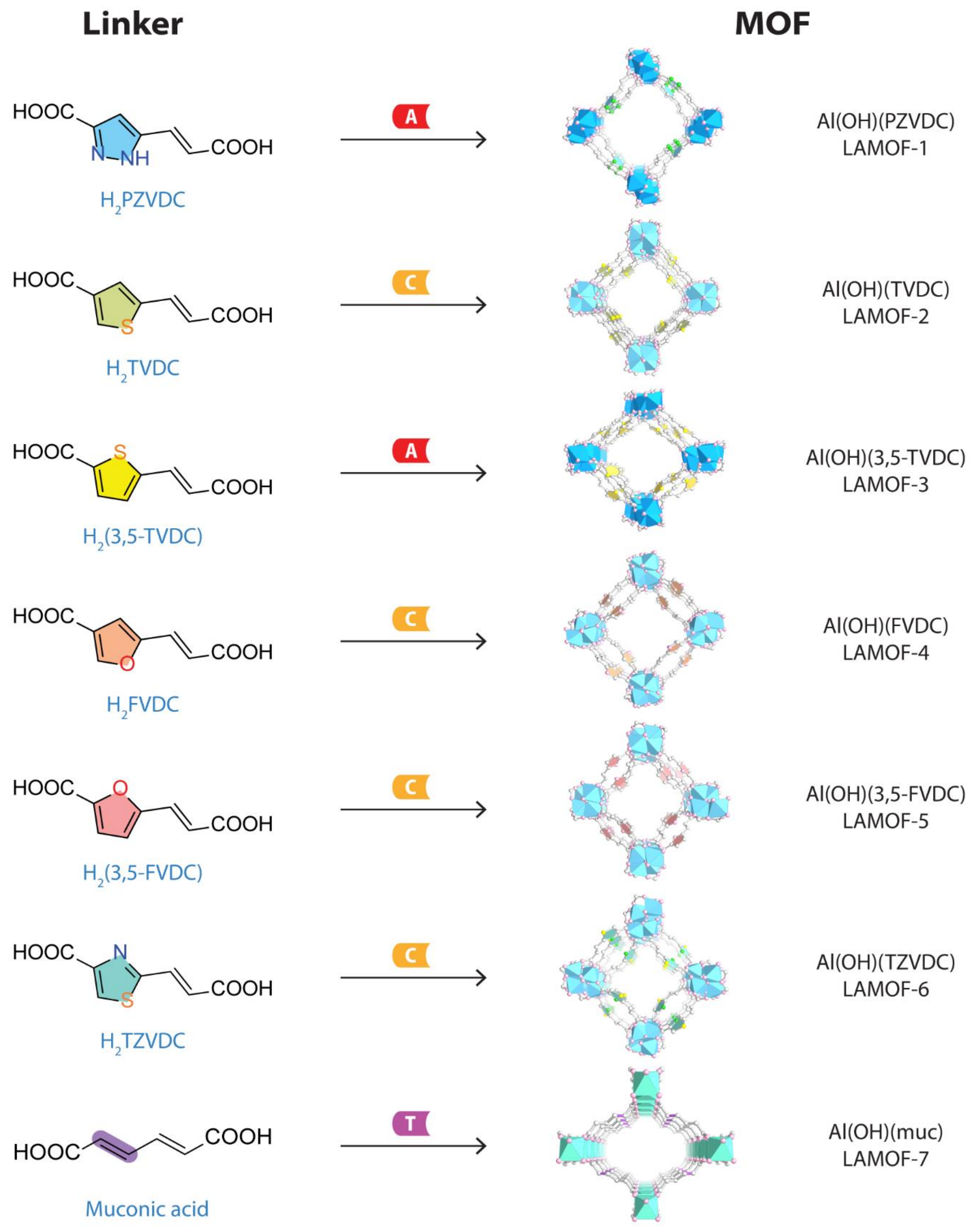
In

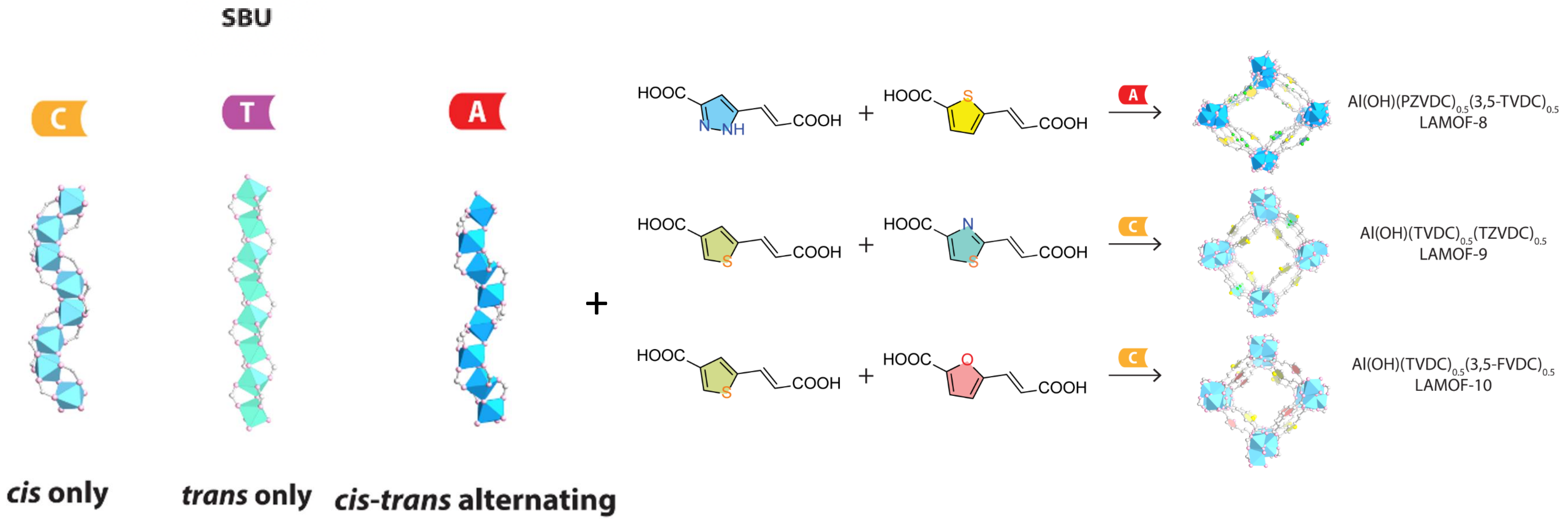
Death Valley

(Furnace Creek)

Shaping the Water Harvesting Behavior by Fine-Tuned GPT Models

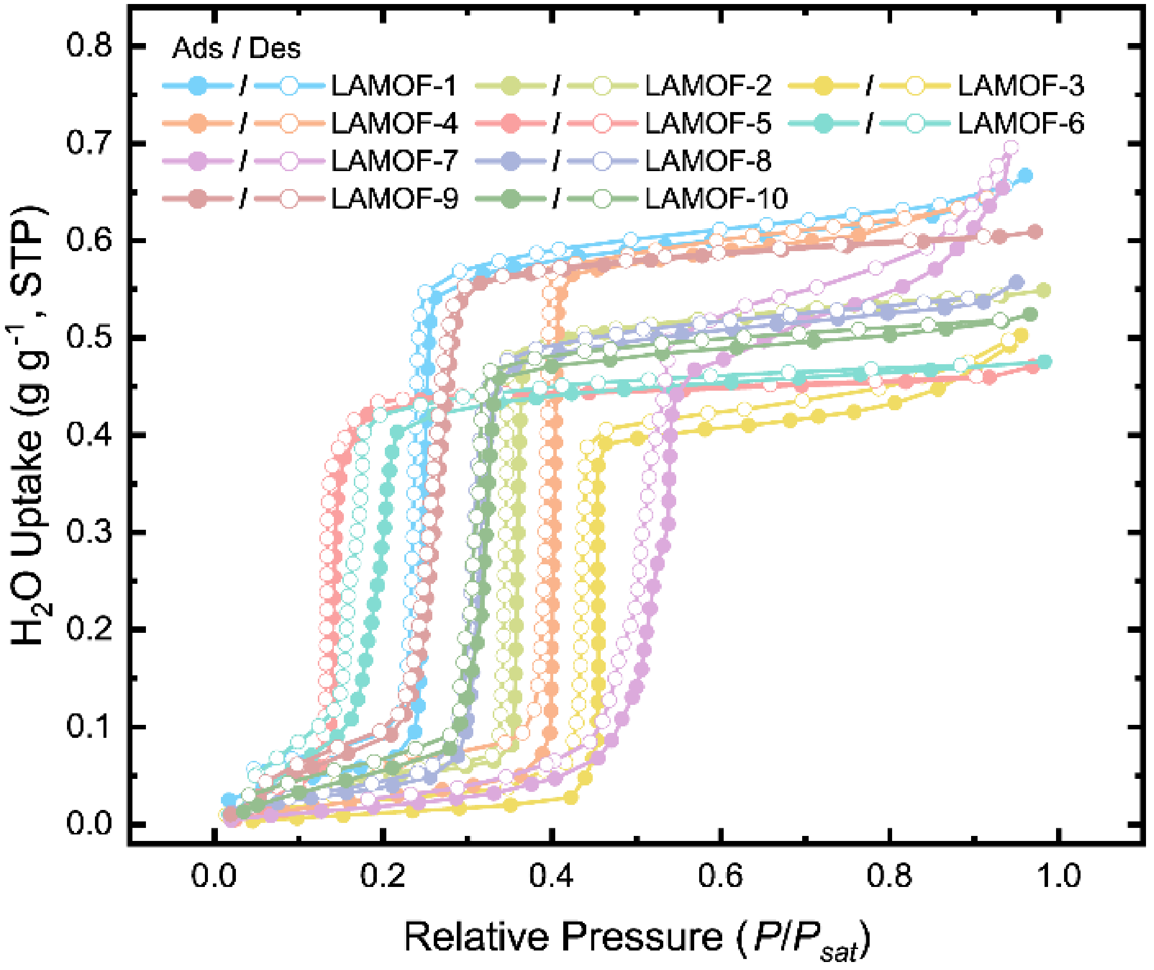


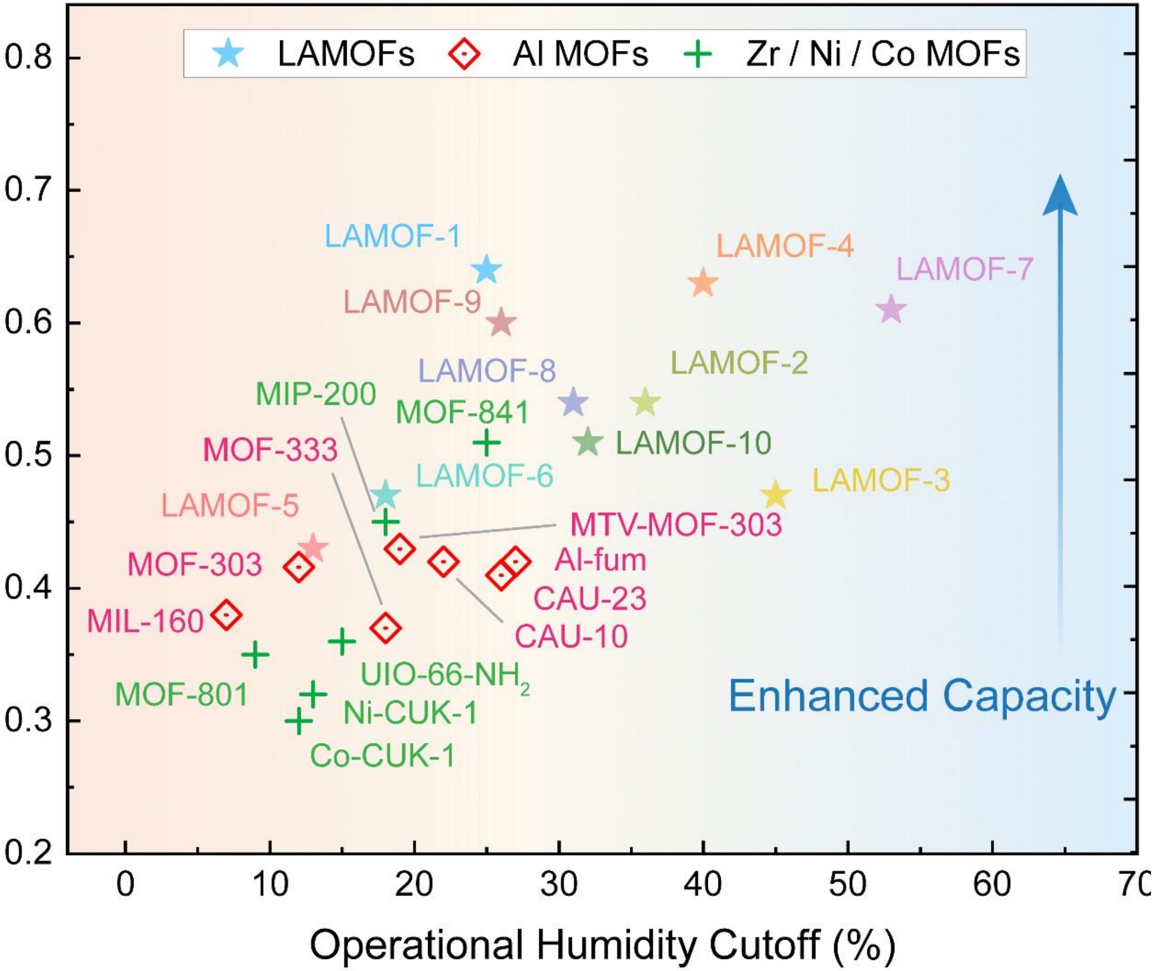




SBU
C
T
A
cis only
trans only
cis-trans alternating
+
HOOC
N
NH
COOH
S
A
C
O
Al(OH)(PZVDC)0.5(3,5-TVDC)0.5
LAMOF-8
Al(OH)(TVDC)0.5(TZVDC)0.5
LAMOF-9
Al(OH)(TVDC)0.5(3,5-FVDC)0.5
LAMOF-10

Shaping the Water Harvesting Behavior Aided GPT Models





Z. Zheng, A. H. Alawadhi, S. Chheda, S. E. Neumann, N. Rampal, S. Liu, H. L. Nguyen, Y. Lin, Z. Rong, J. I. Siepmann, L. Gagliardi, A. Anandkumar, C. Borgs, J. T. Chayes, O. M. Yaghi, *J. Am. Chem. Soc.*, **2023**, *145*, 28284–28295.

On-Grid Water Harvester – Planned First Commercial Release

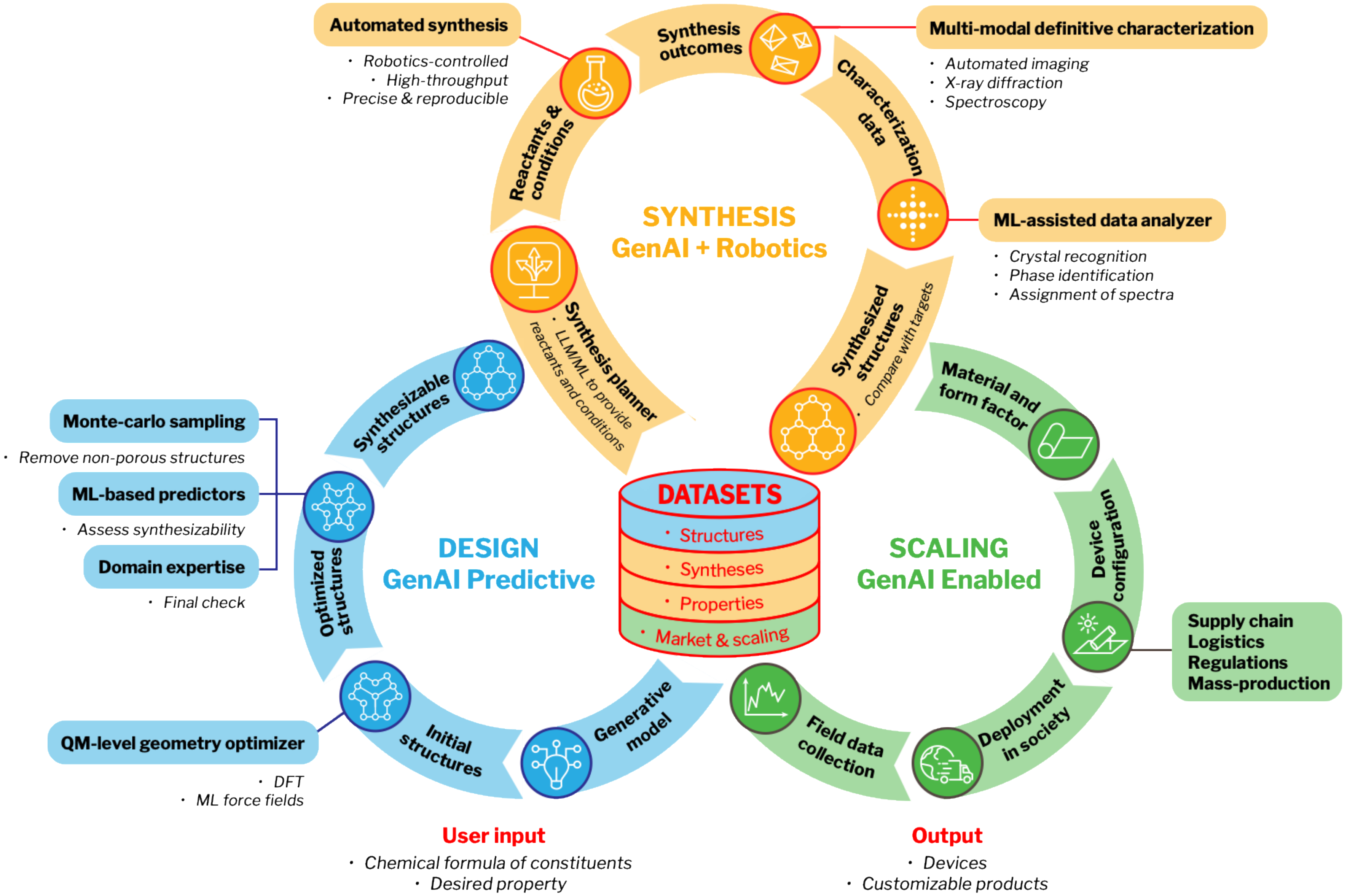
Ambient RH	Ambient Temp. (°C)	Daily Capacity (Liters)	Avg. Energy Consumption (kWh/L)
40%	25	~ 2,000	0.3
25%	25	~ 2,000	0.4
15%	25	~ 2,000	0.6

Off-Grid Water Harvester

Ambient RH	Ambient Temp. (C)	Temp. of Thermal Input (°C)	Daily Capacity (Liters)
30%	25	70	~ 850
30%	25	60	~ 600

A platform for molecule to society

A Platform for Molecule to Society



Zichao Rong

Better, cheaper, faster, and greener

Crystal structures of ZIFs and LZIFs discovered

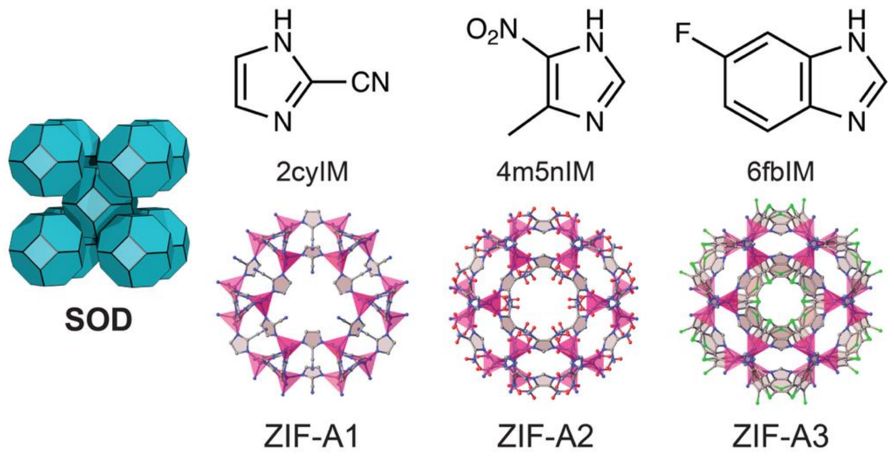
- Dataset of 2,688 reactions across 8 ZIF linkers. Machine learning methodology achieved:

Twice the discovery rate (number of crystals per experiment) of random exploration.

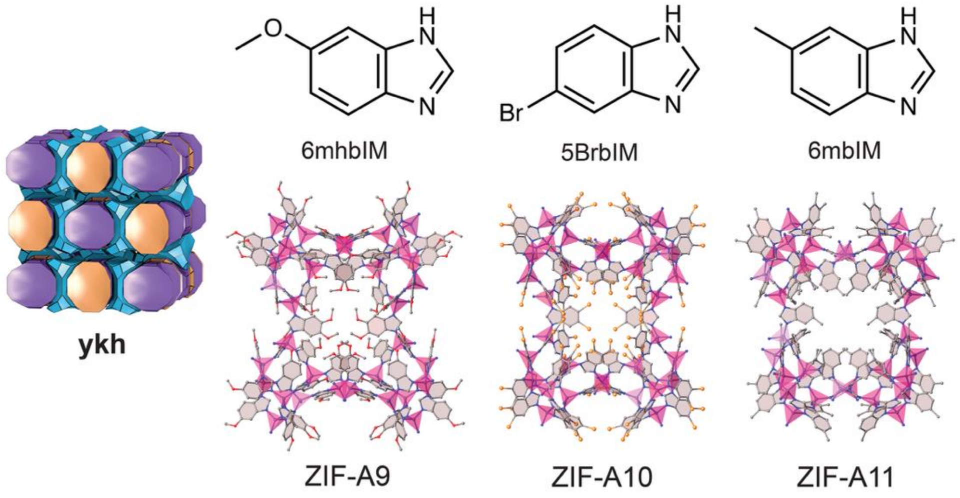
- Dealing with small number of data:

Encode the data by introducing chemistry intelligent descriptors.

Simplify the model by choosing the best most adaptive architecture.



Expected structures



Unexpected structures

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Yue-Biao Zhang
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