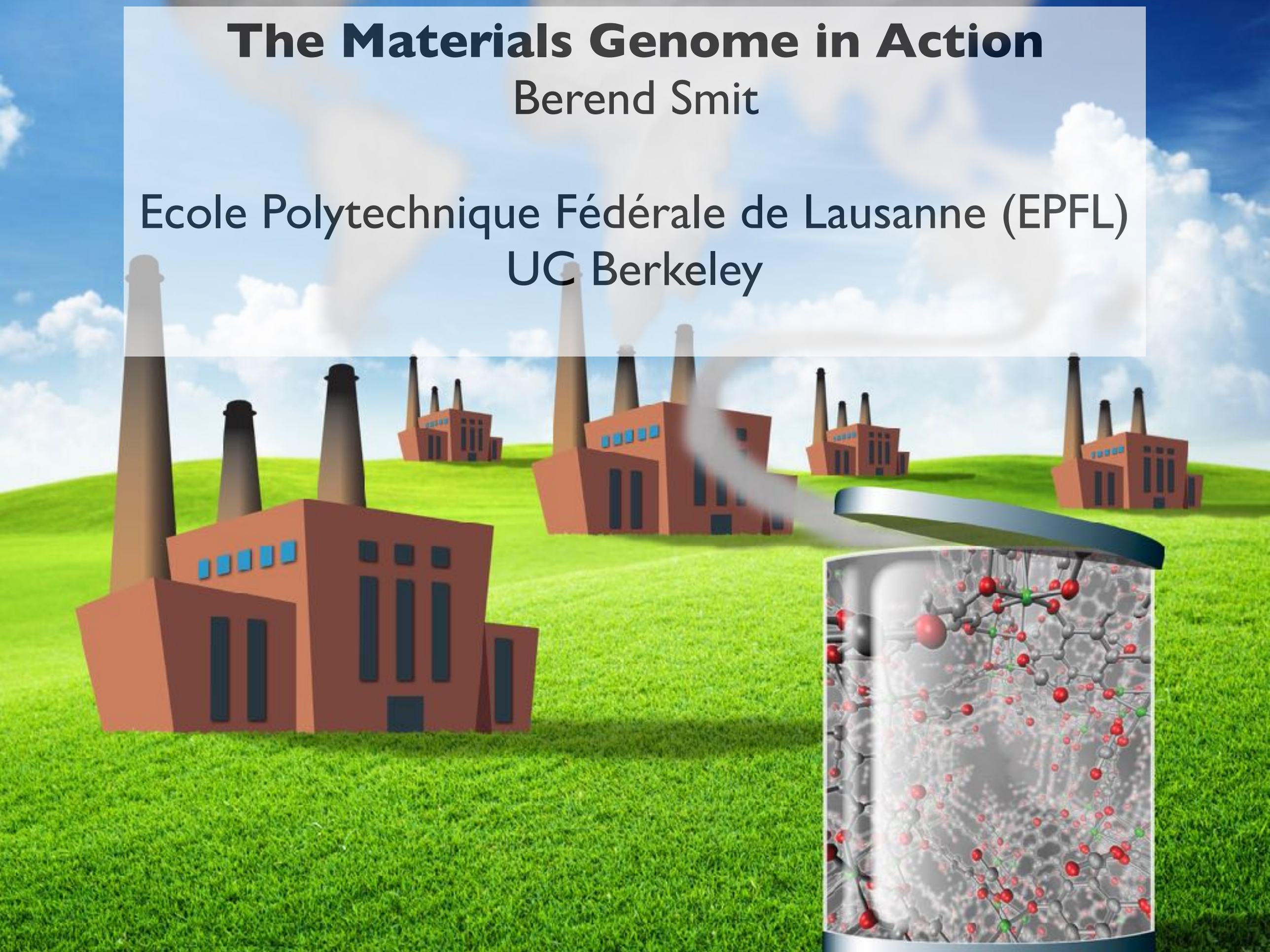
The Materials Genome in Action

Berend Smit

Ecole Polytechnique Fédérale de Lausanne (EPFL)
UC Berkeley



Outline

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- The Materials Genome

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- Materials for Xe/Kr separations
  - a short success story

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- A Theory of Nothing
  - example of mean science
  - back to methane storage

Acknowledgement

- **Materials Genome**
  - Cory Simon, Matt Witman and Rocio Mercado (UC Berkeley)
  - Kyriakos Stylianou (EPFL)
  - Jihan Kim (KAIST), Michael Deem (Rice), Maciej Haranczyk (LBNL), David Sholl (GeorgiaTech), Randy Snurr (Northwestern)
- **Similarity**
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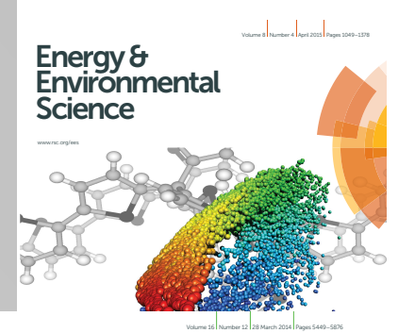
  - Pawel Dlotko (Inria France)
- **Financial Support**
  - ERC-Adv, US Department of Energy, MARVEL (NCCR-SNF)



CGS | Center for Gas Separations Relevant to Clean Energy Technologies

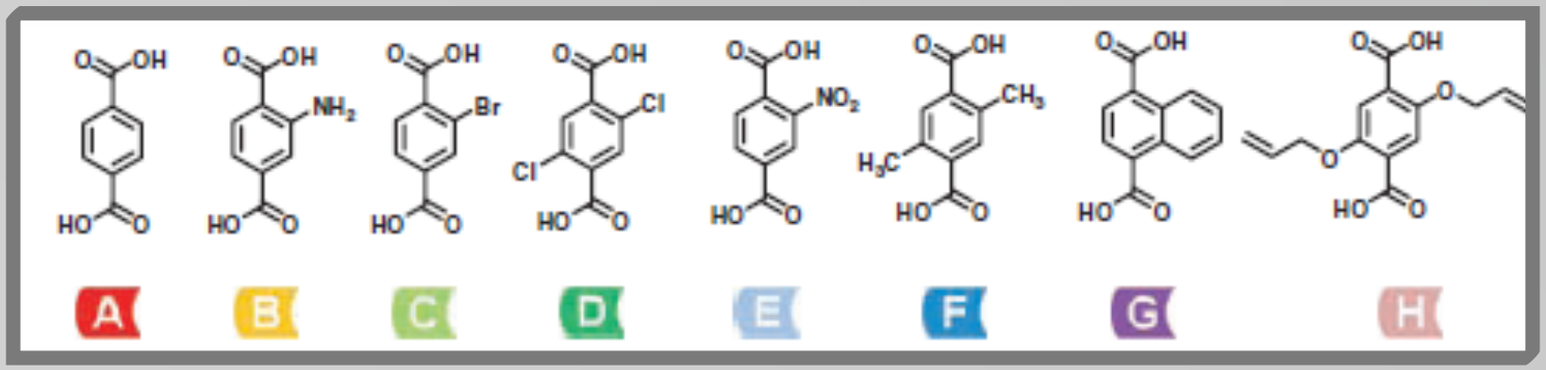
erc European Research Council

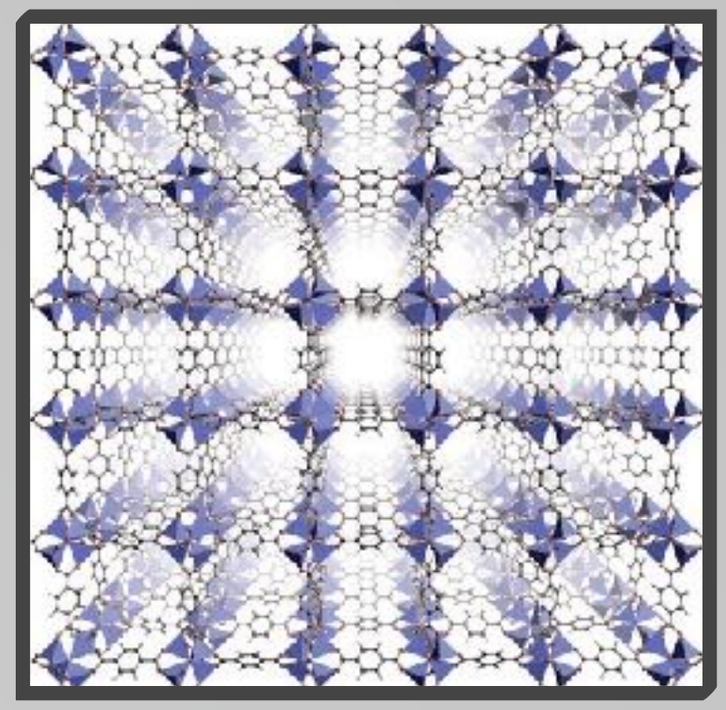
FNSNF

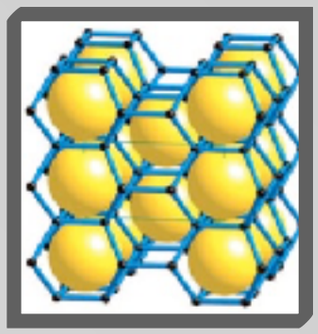
MARVEL

The Material Genome

Computation Challenge







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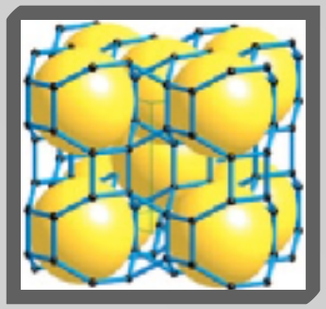

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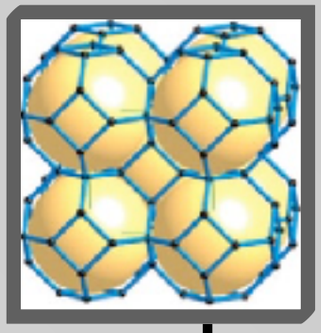

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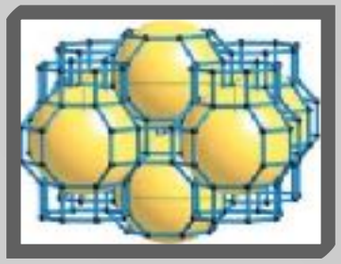

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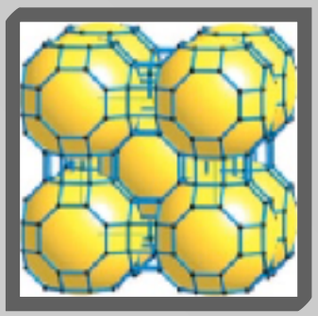

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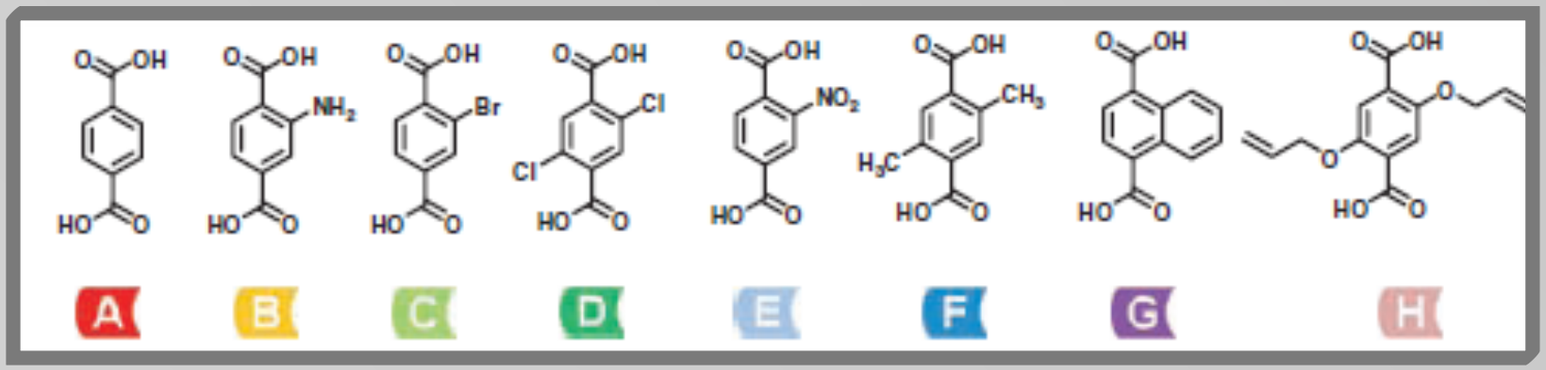
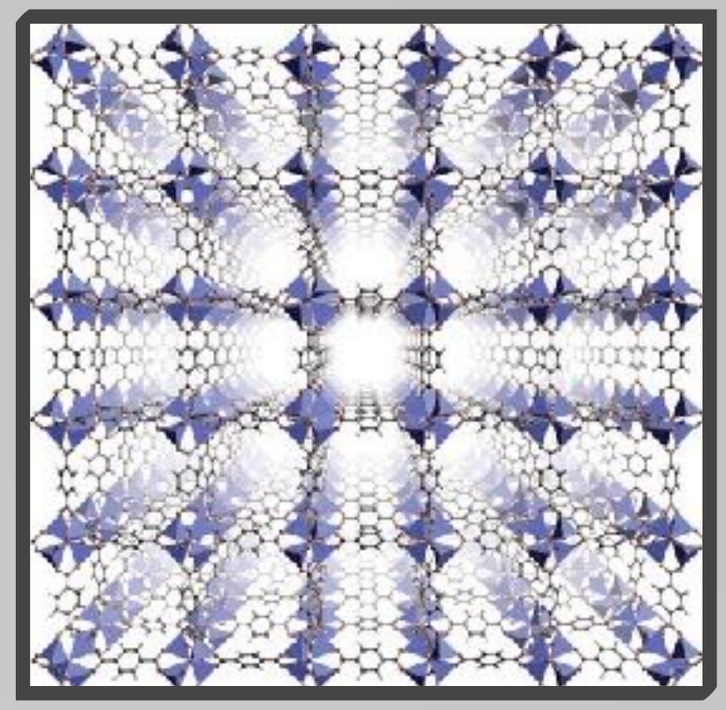
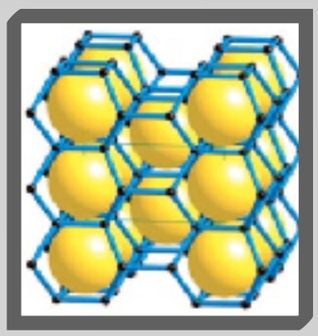
Computation Challenge

Chemical Flexibility of MOFs







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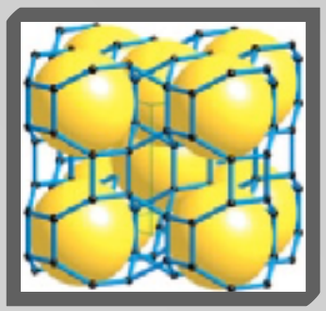

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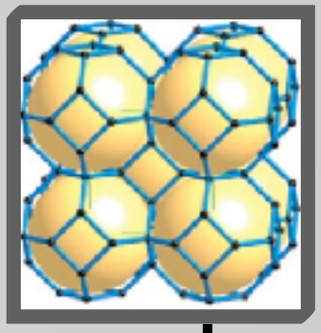

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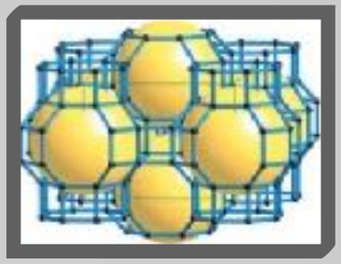

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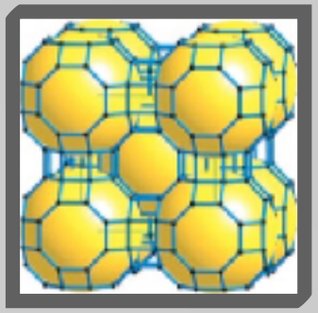

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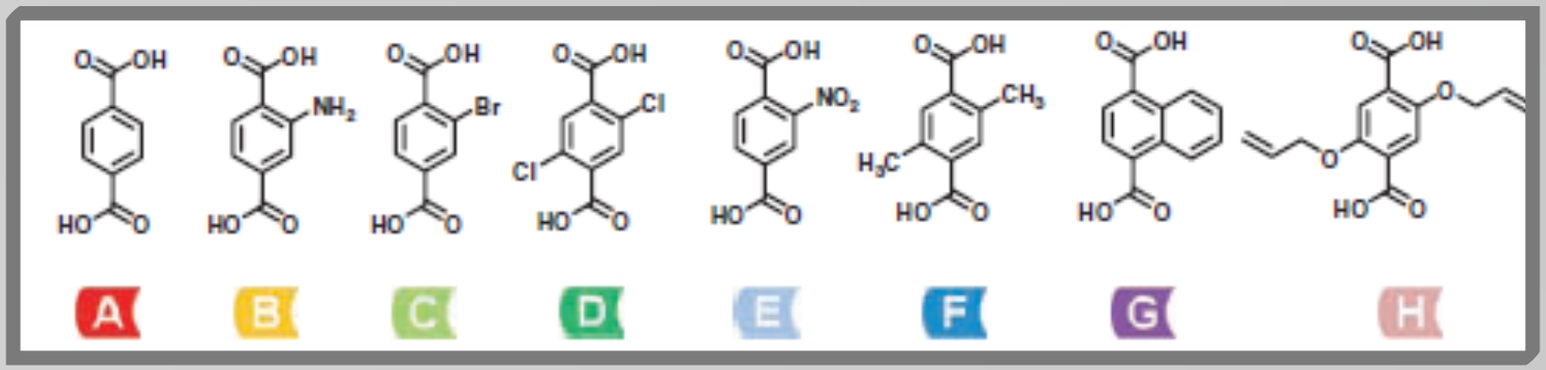

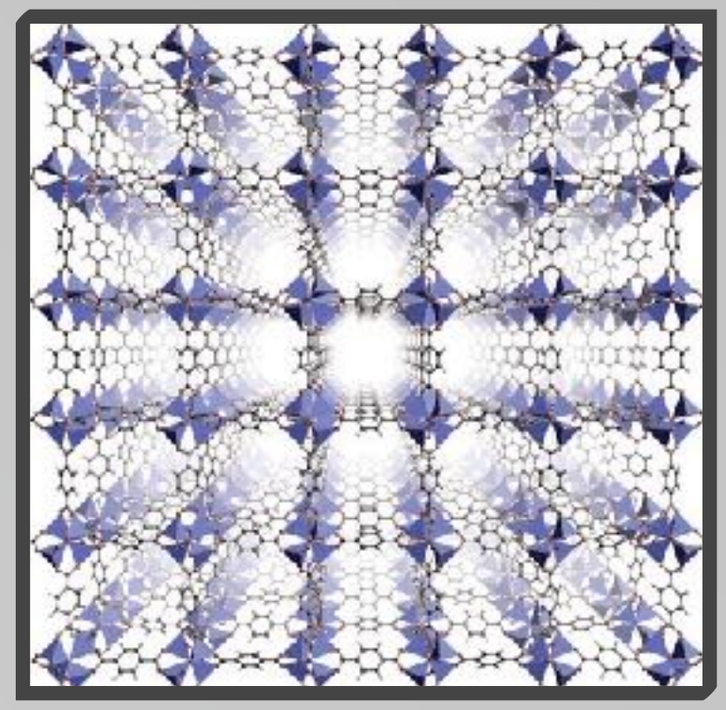

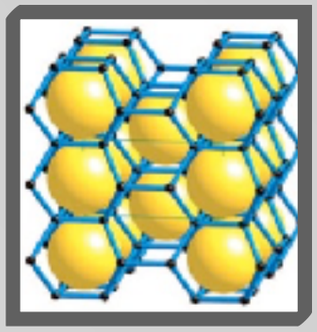

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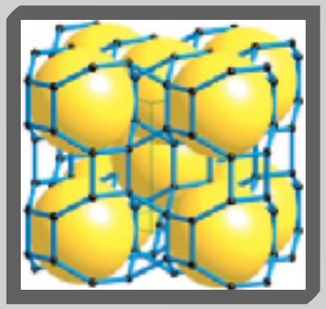

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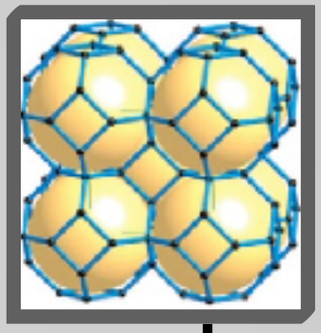

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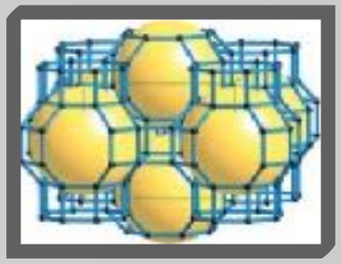

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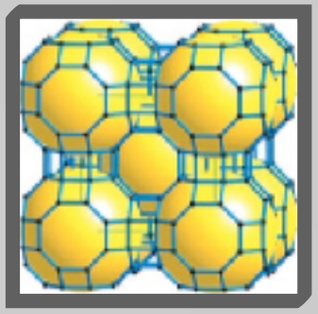

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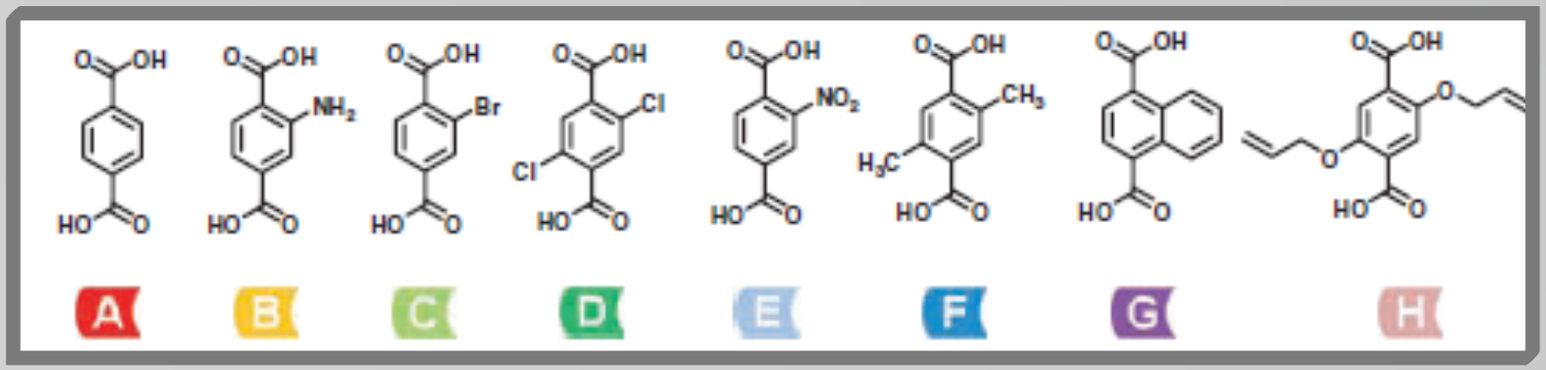

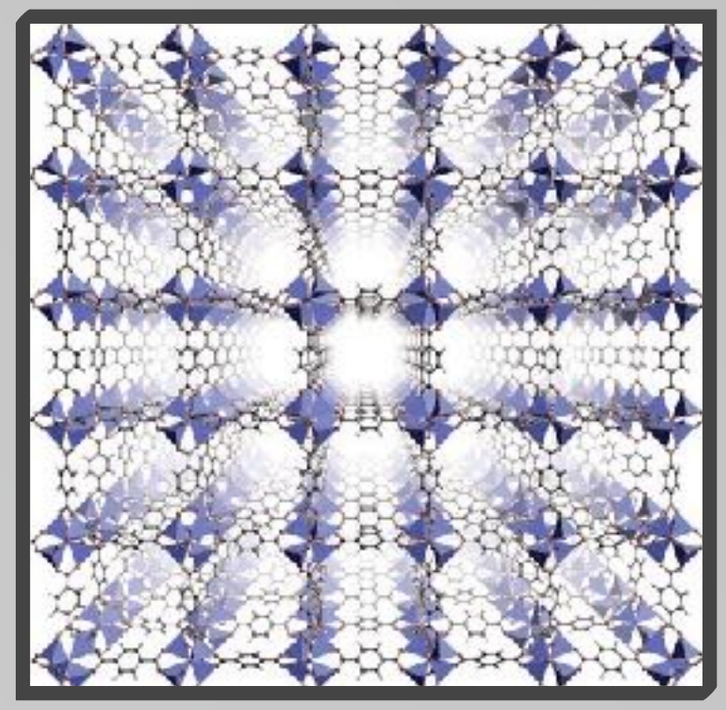

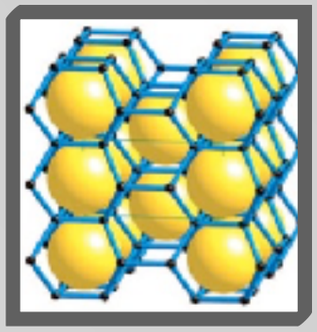

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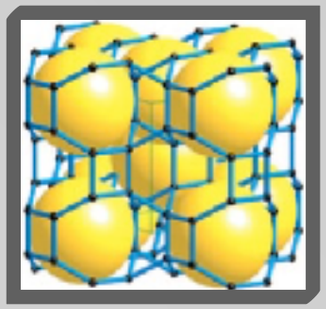

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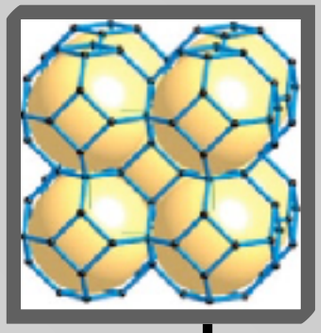

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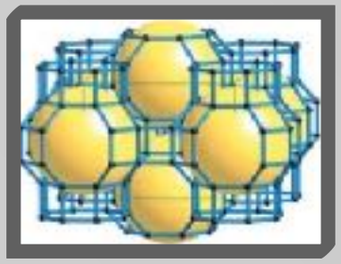

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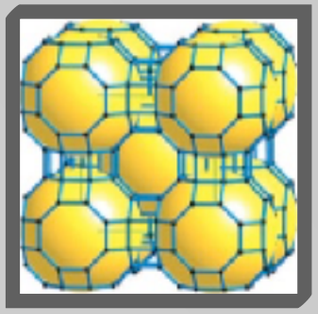

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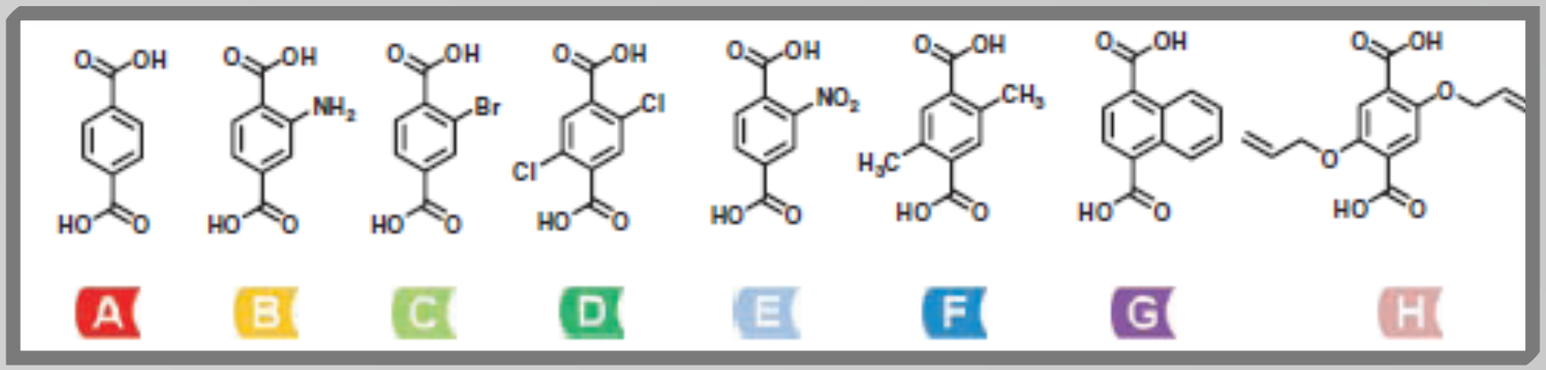

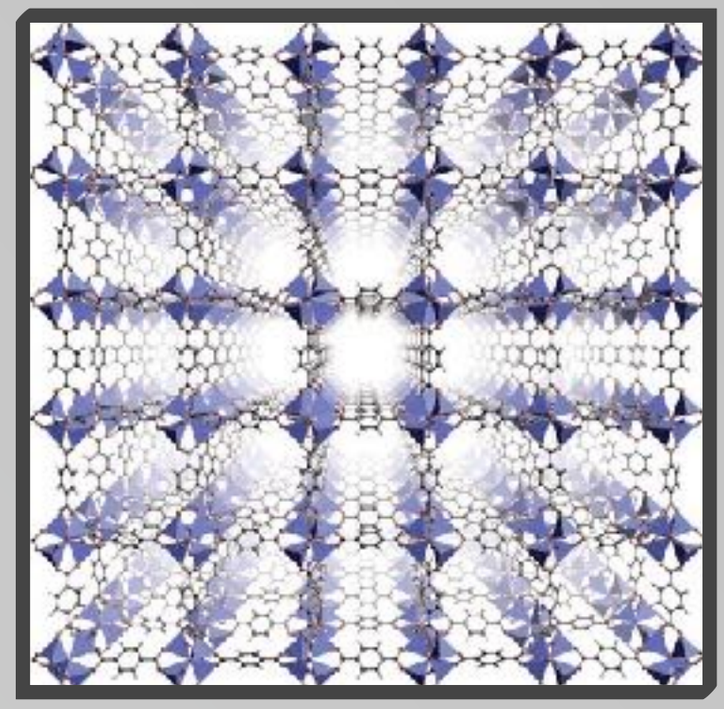

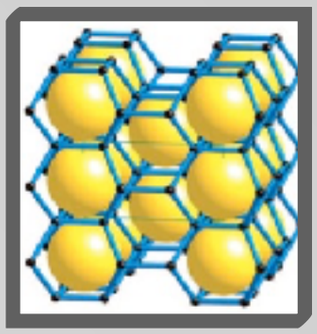

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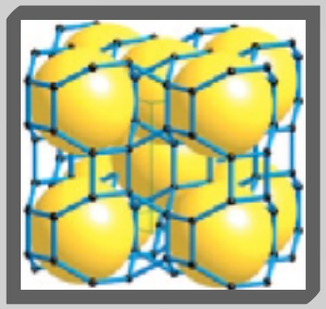

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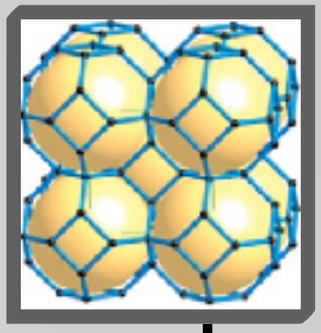

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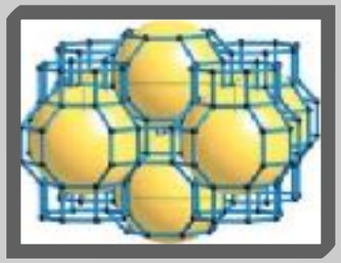

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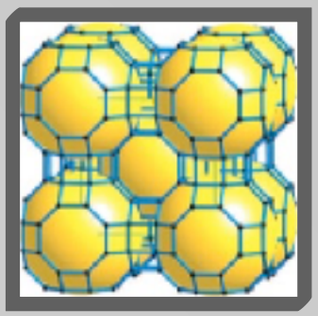

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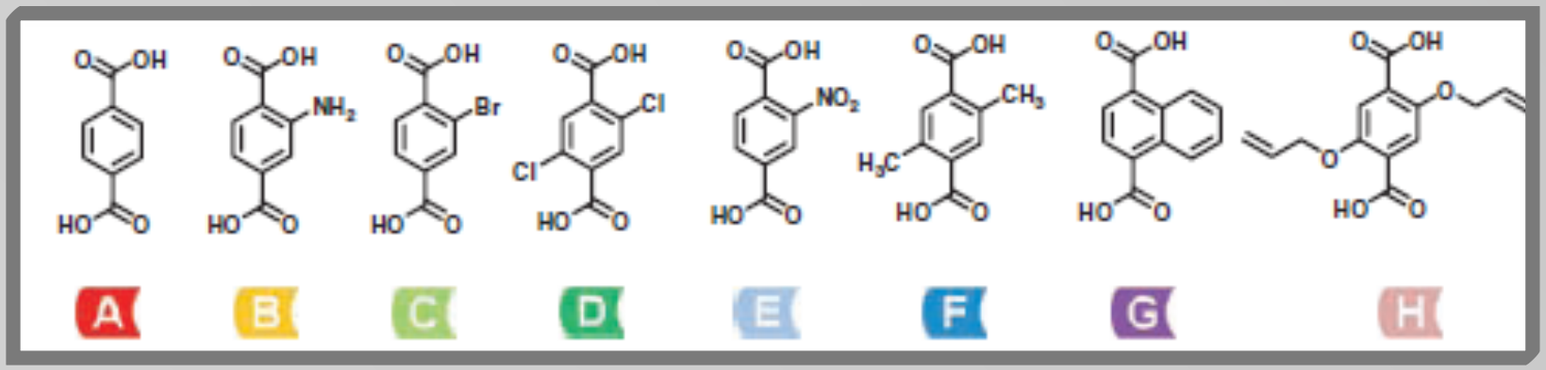

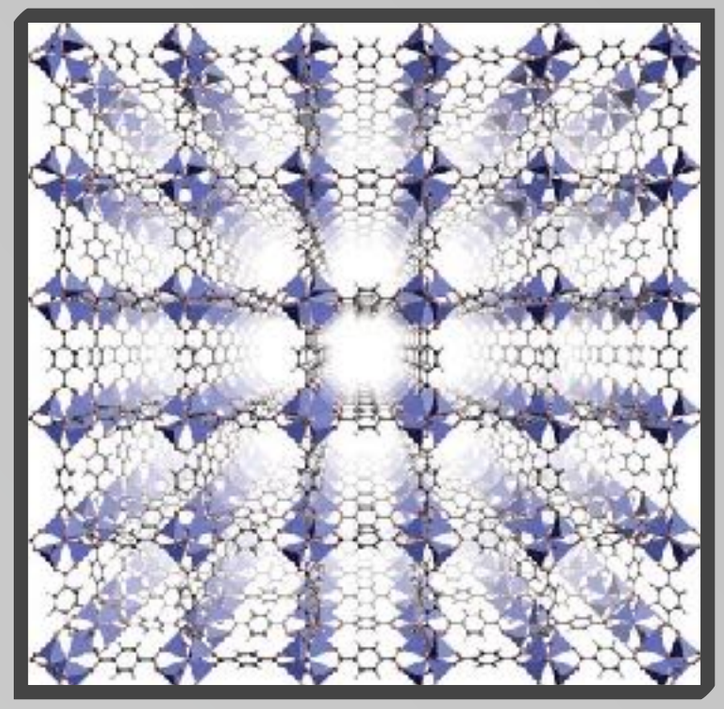

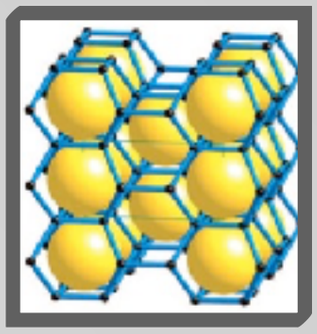

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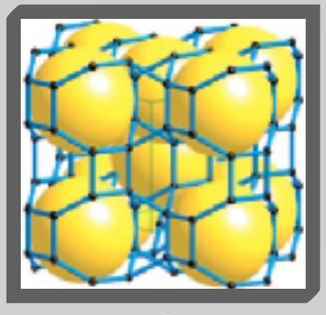

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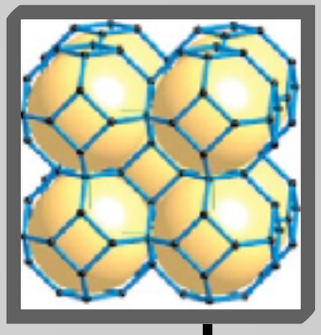

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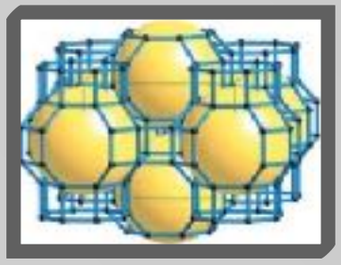

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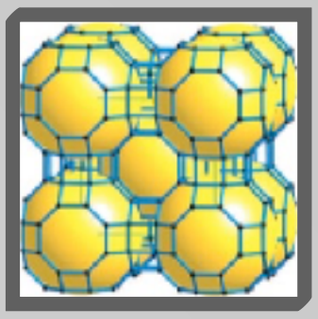

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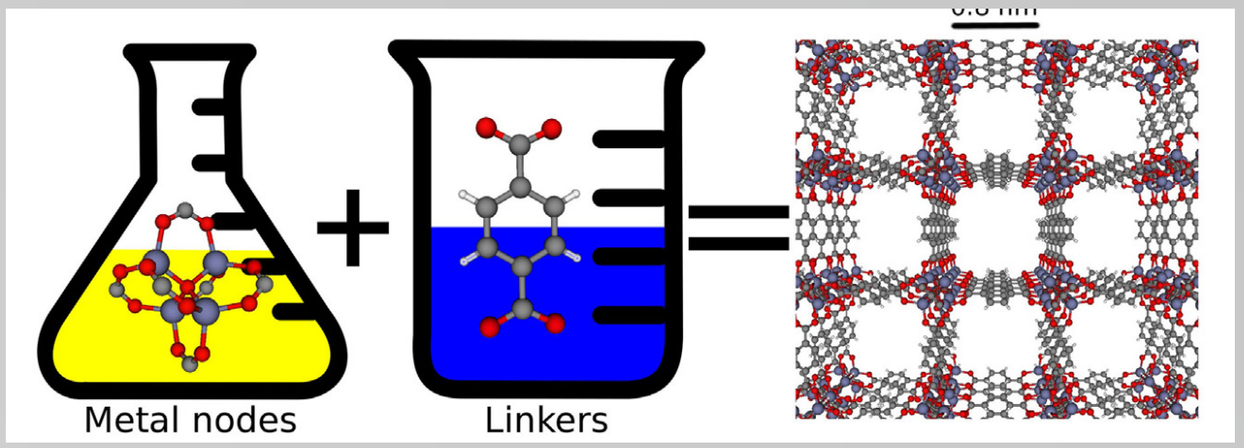
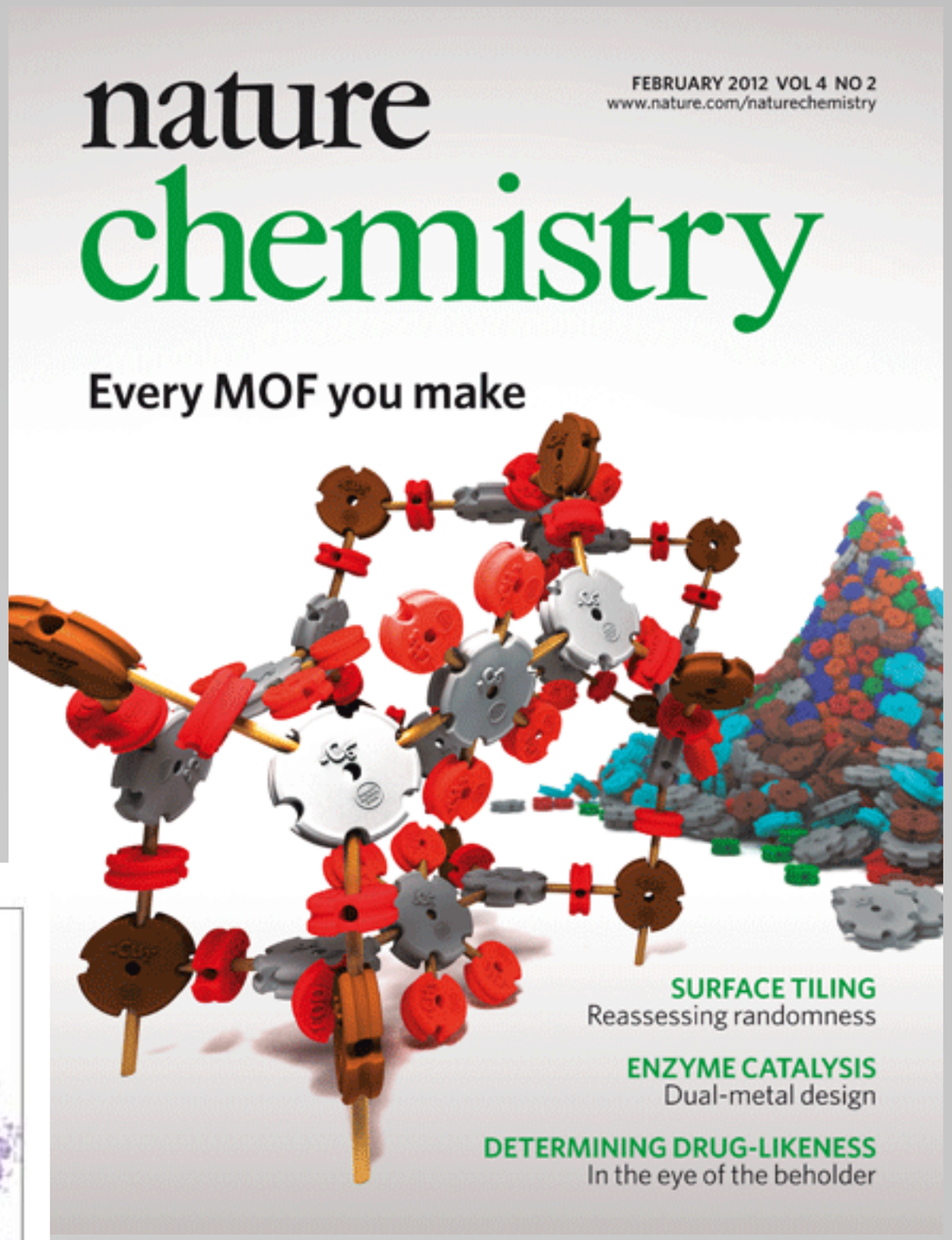
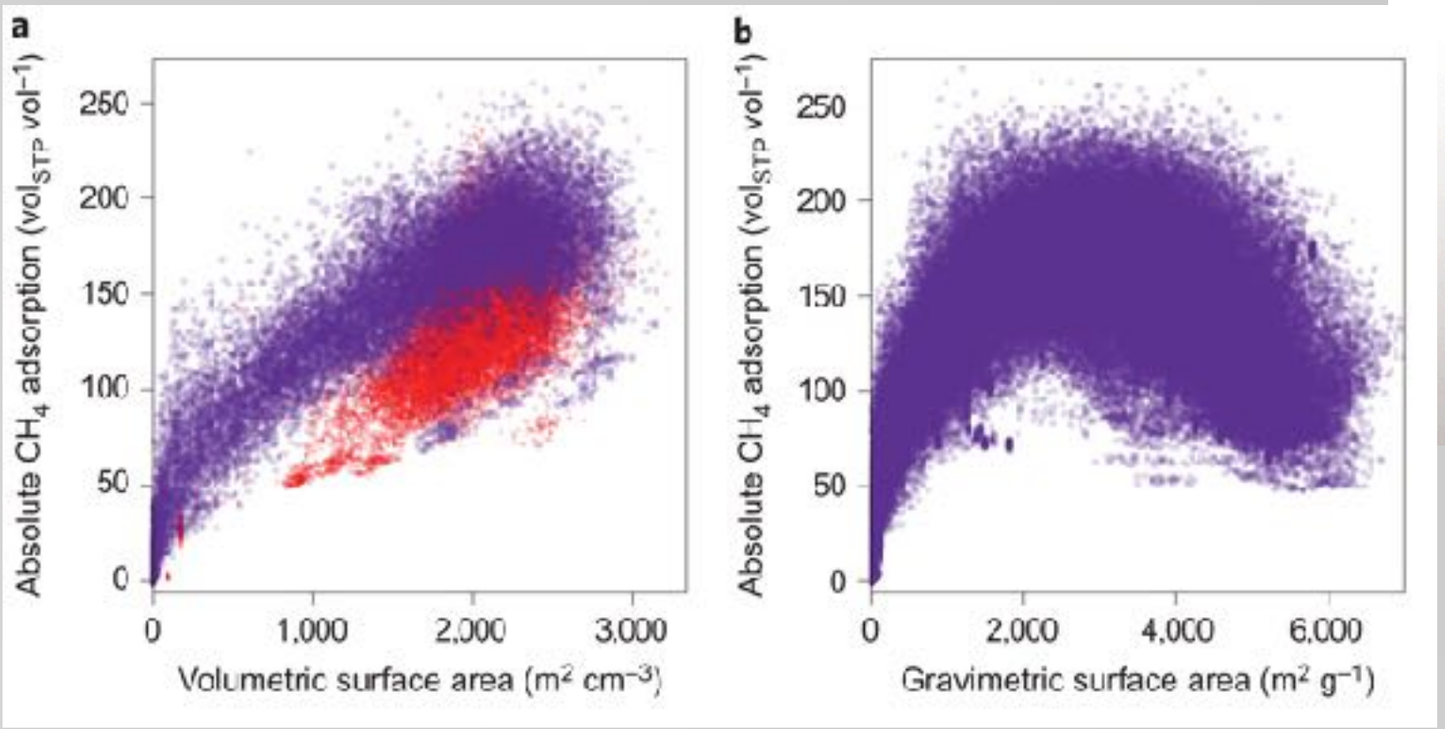
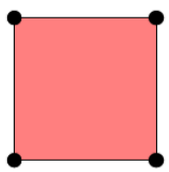
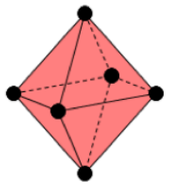
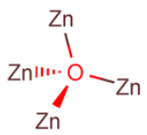
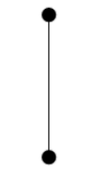
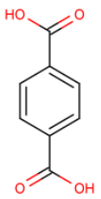
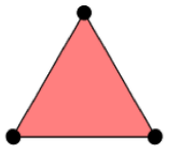
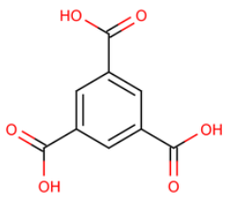
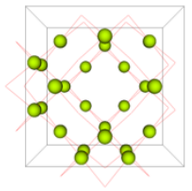
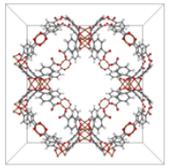
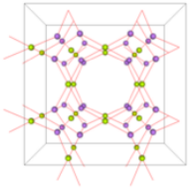
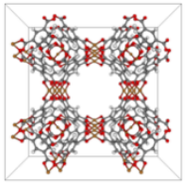
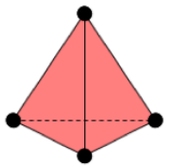
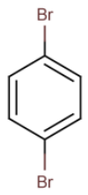
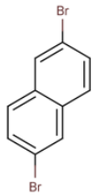
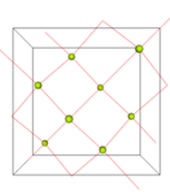
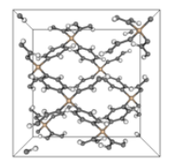
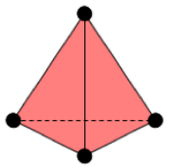
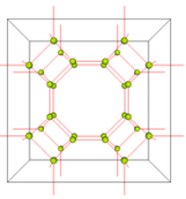
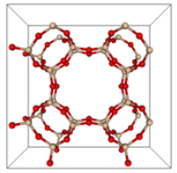
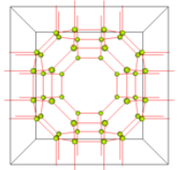
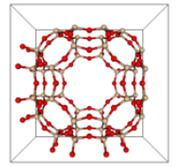
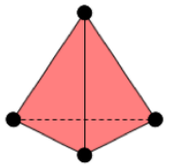
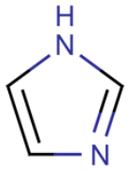
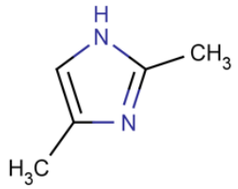
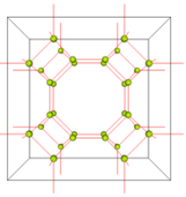
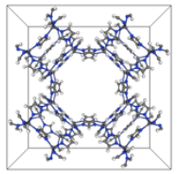
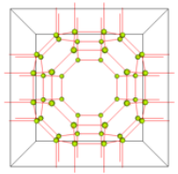
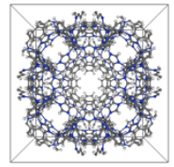
Out of these many many millions of structures, which one is the best for a given applications?





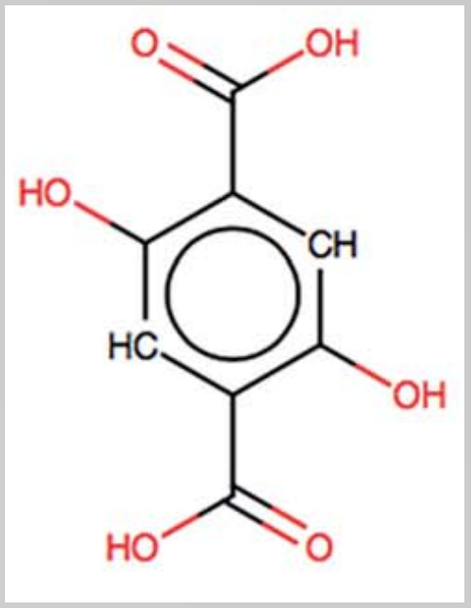


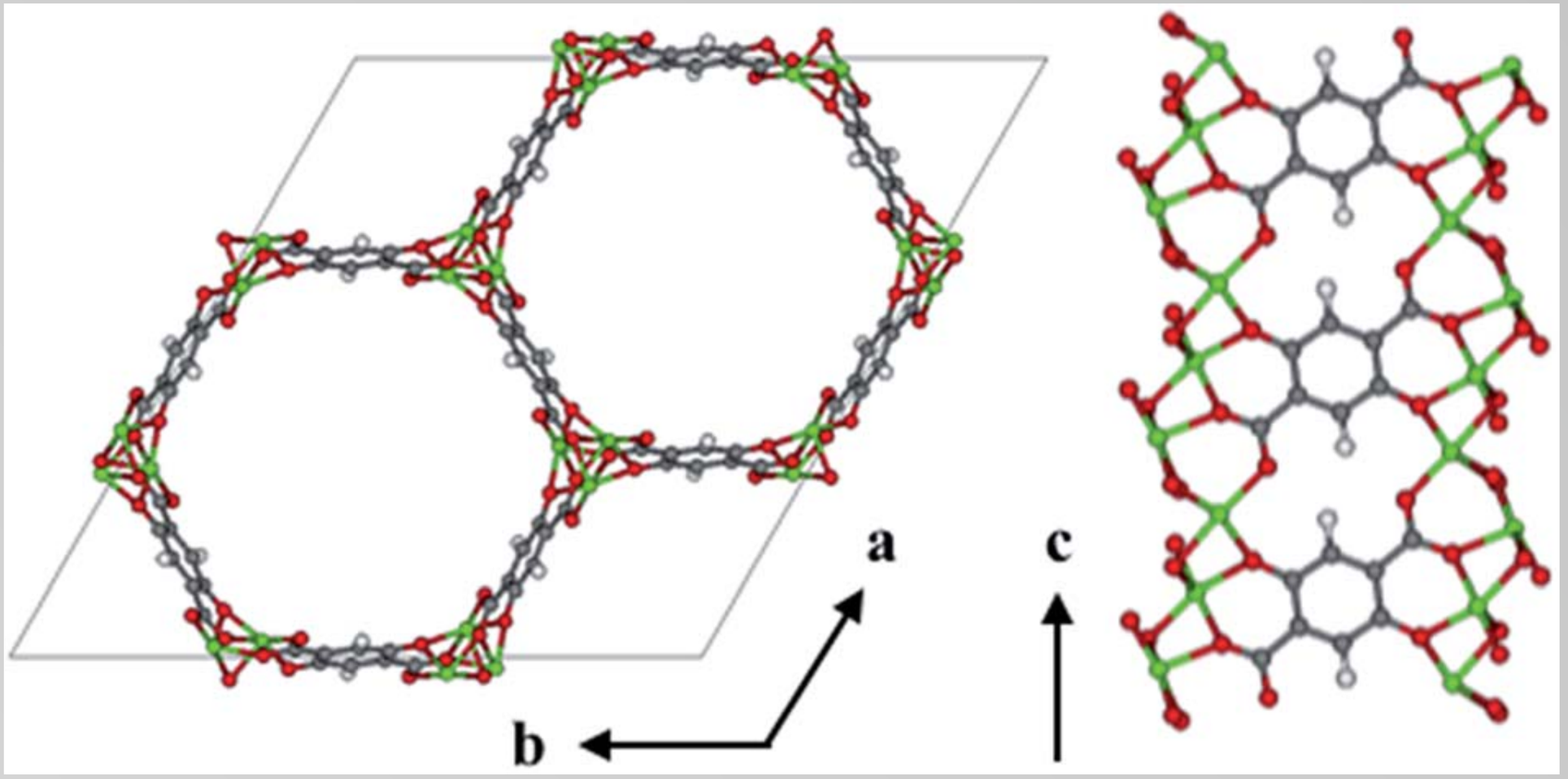
C. E. Wilmer, M. Leaf, C. Y. Lee, O. K. Farha, B. G. Hauser, J. T. Hupp, R. Q. Snurr, *Nat Chem* **2012**, *4*, 83-89.

Material class	Building blocks				Topologies	
MOFs	 Cu—Cu	 	 	 	 	 
PPNs	 Si	Ge			 	
Zeolites	 Si		O		 	 
ZIFs	 Zn	Fe			 	 

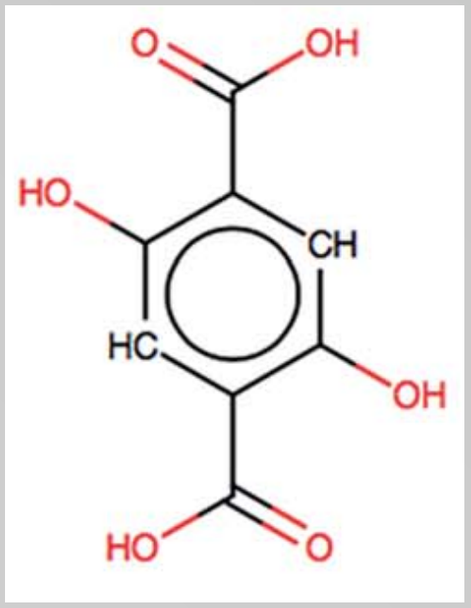
> 3,000,000 materials

Mg MOF-74

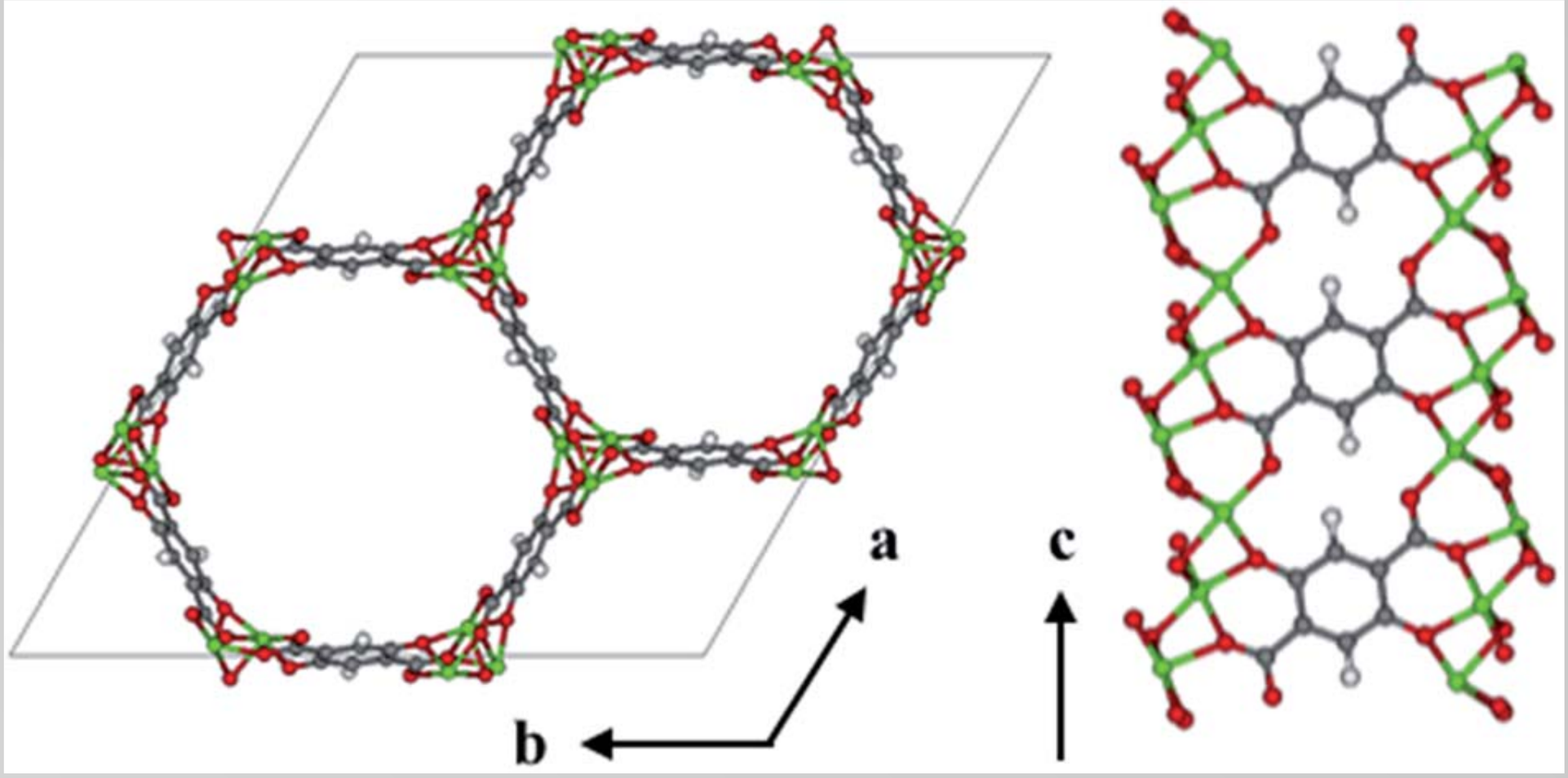




Mg MOF-74



Question: how many Mg-MOF-74 can we synthesize using known chemicals?

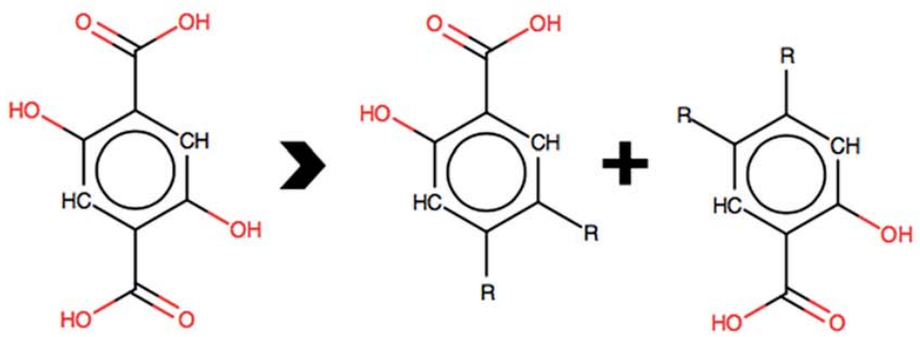


In silico generation of MOF-74 analogs

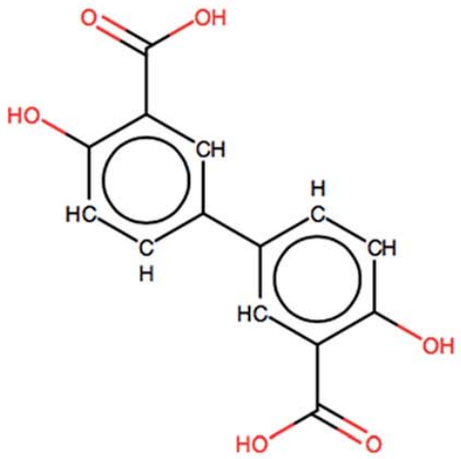
Filter step (Remaining potential ligands)

(1) Database Selection (~ 60,000,000)

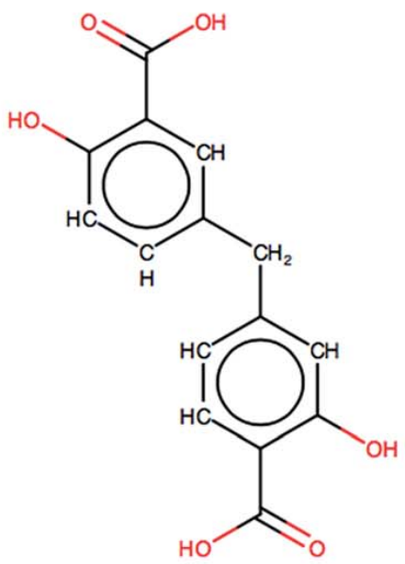
(2) Connectivity Filter (~ 400):



(3) High Energy Conformer Filter (61):



CAN satisfy low energy conformer requirements



CANNOT satisfy low energy conformer requirements

M. Witman, et al Chem. Sci**. 7** (9), 6263 (2016) http://dx.doi.org/10.1039/c6sc01477a

In silico generation of MOF-74 analogs

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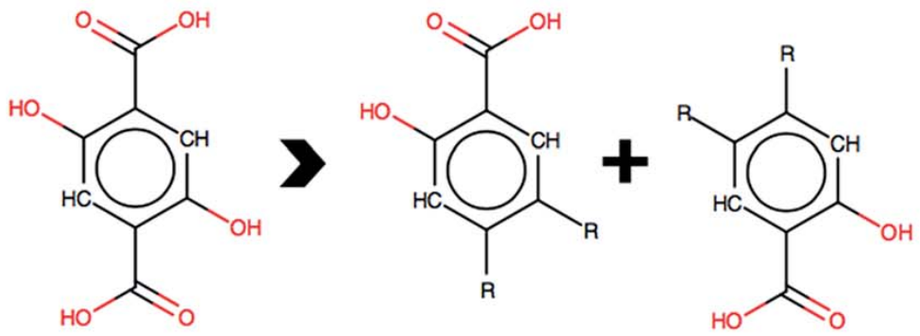
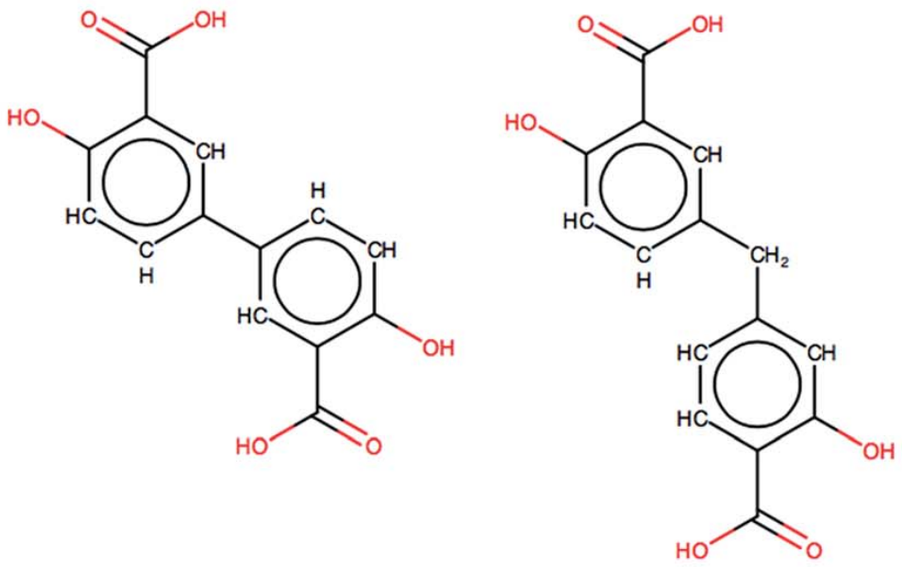
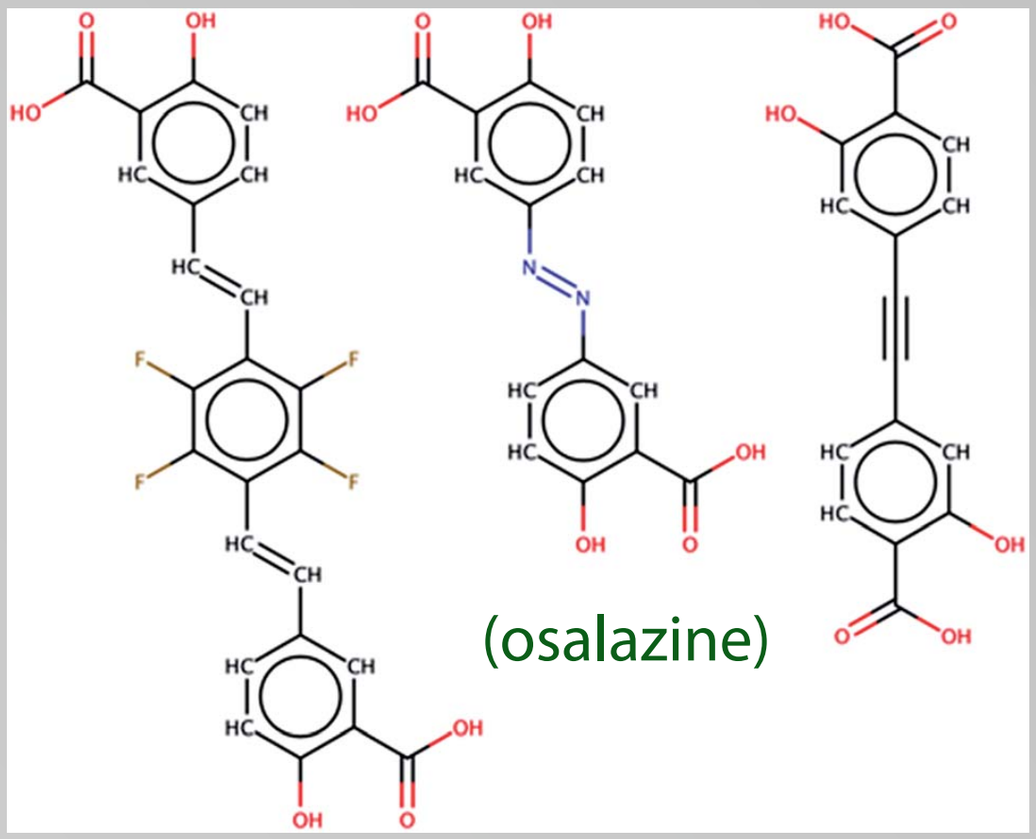


(3) *High Energy Conformer Filter* (61):



CAN satisfy low energy conformer requirements

CANNOT satisfy low energy conformer requirements



(osalazine)

M. Witman, et al Chem. Sci**. 7** (9), 6263 (2016) http://dx.doi.org/10.1039/c6sc01477a

In silico generation of MOF-74 analogs

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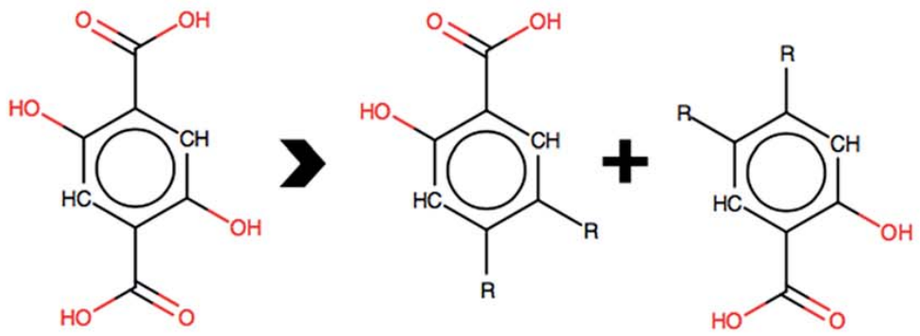
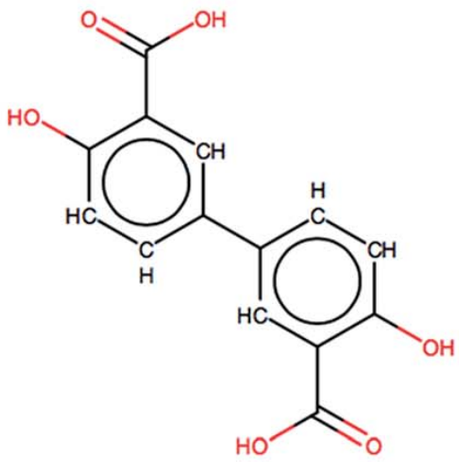
(1) *Database Selection* (~ 60,000,000)

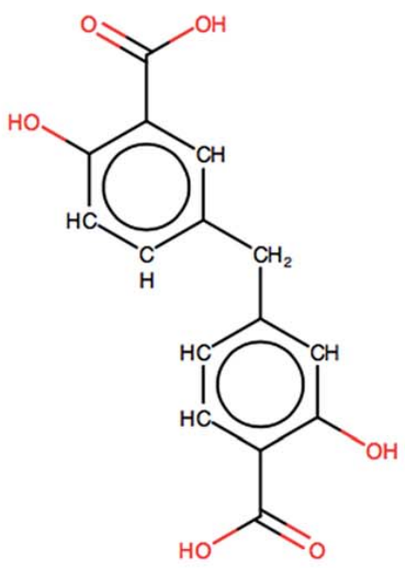
(2) *Connectivity Filter* (~ 400):



(3) *High Energy Conformer Filter* (61):



CAN satisfy low energy conformer requirements



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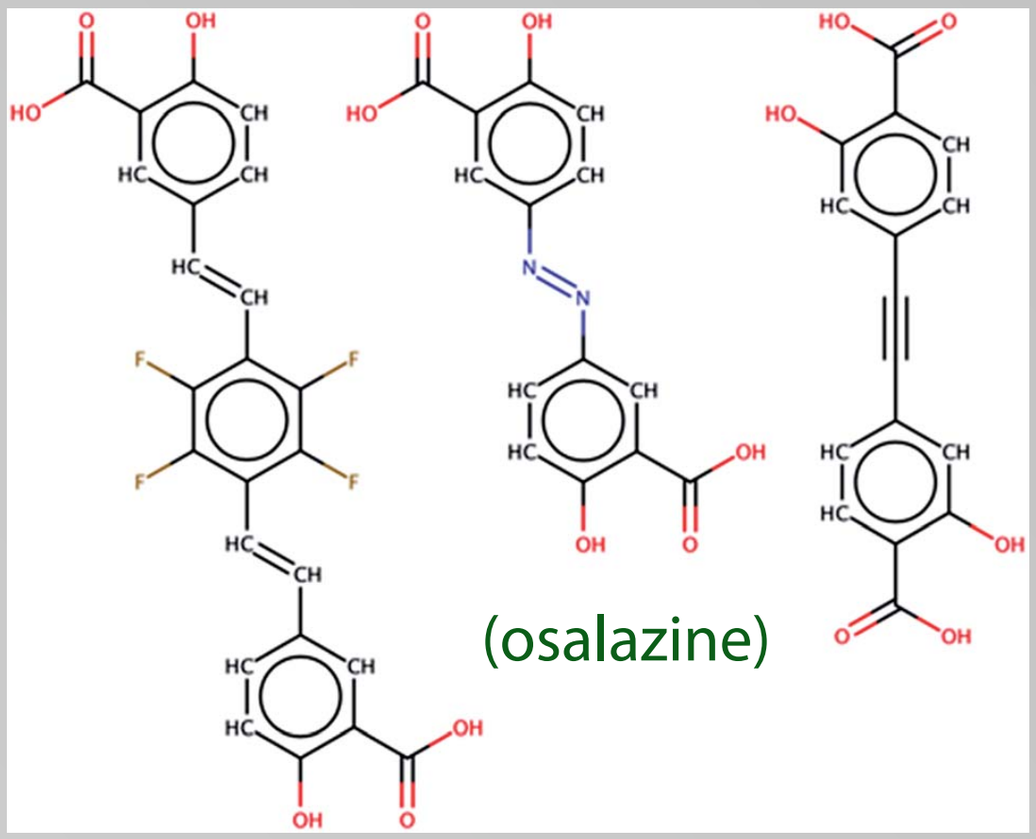
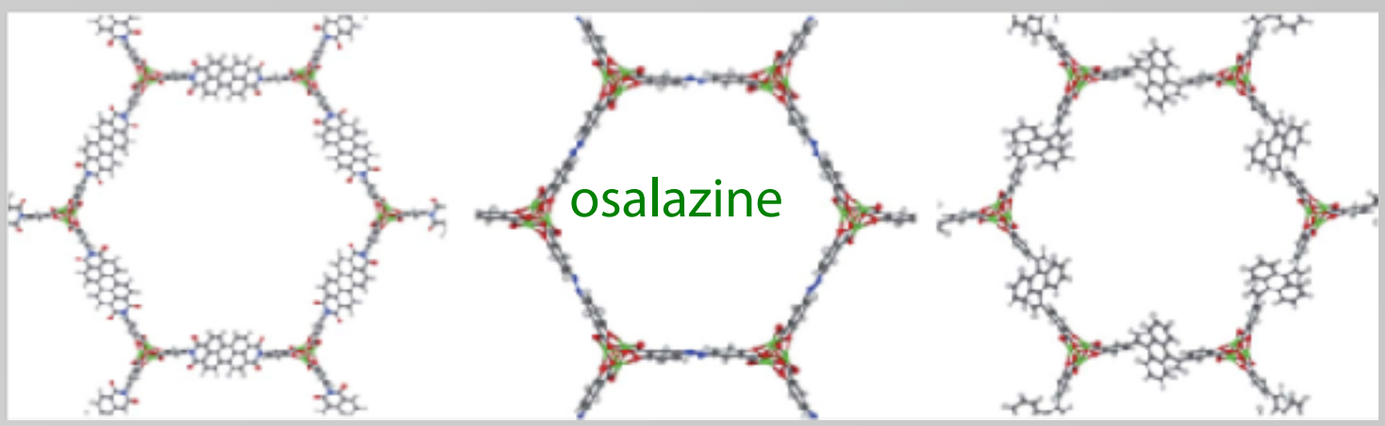
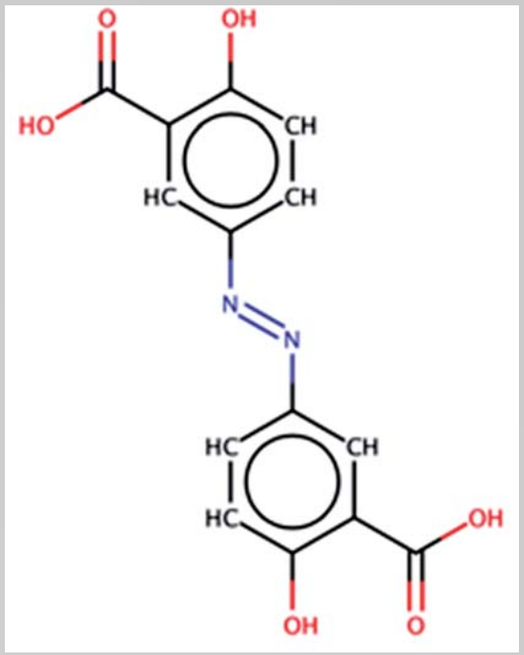
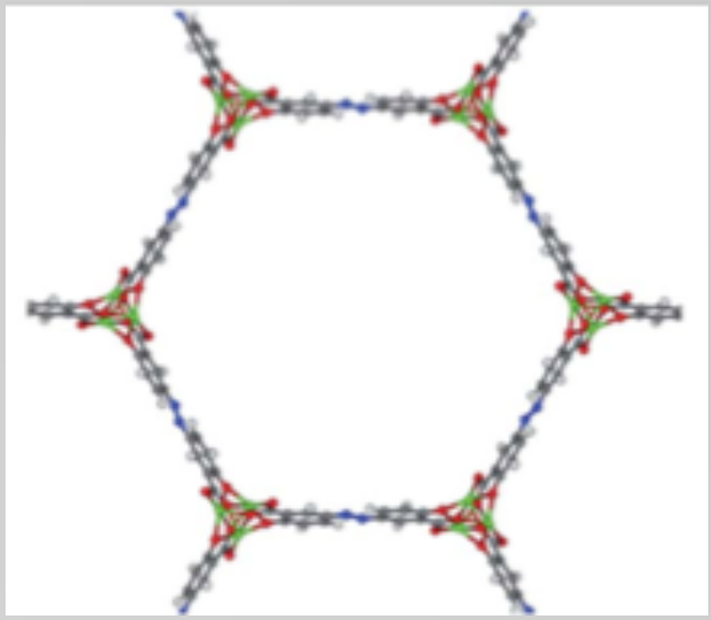




M. Witman, et al Chem. Sci. **7** (9), 6263 (2016) http://dx.doi.org/10.1039/c6sc01477a

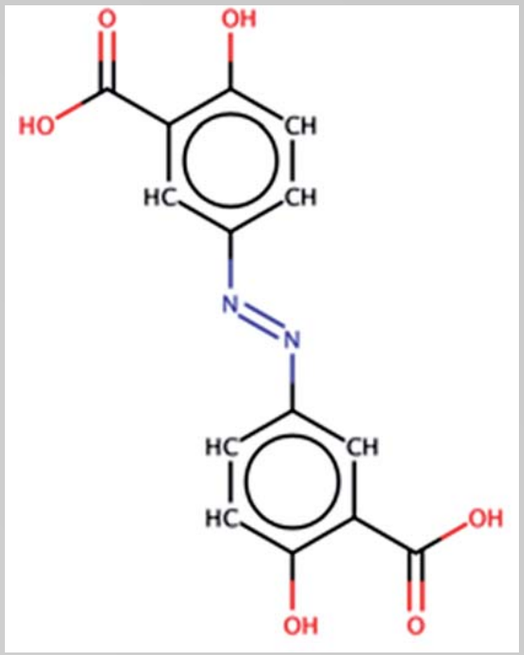
Mg-MOF-74 osalazine

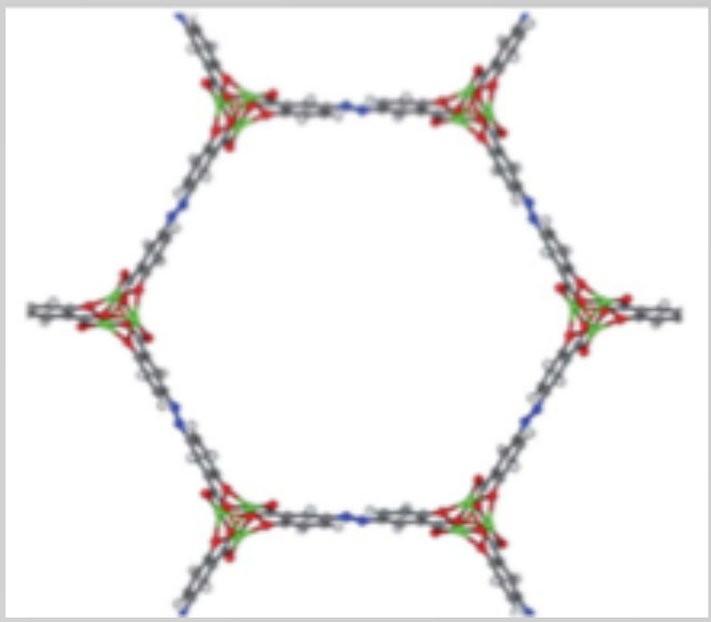


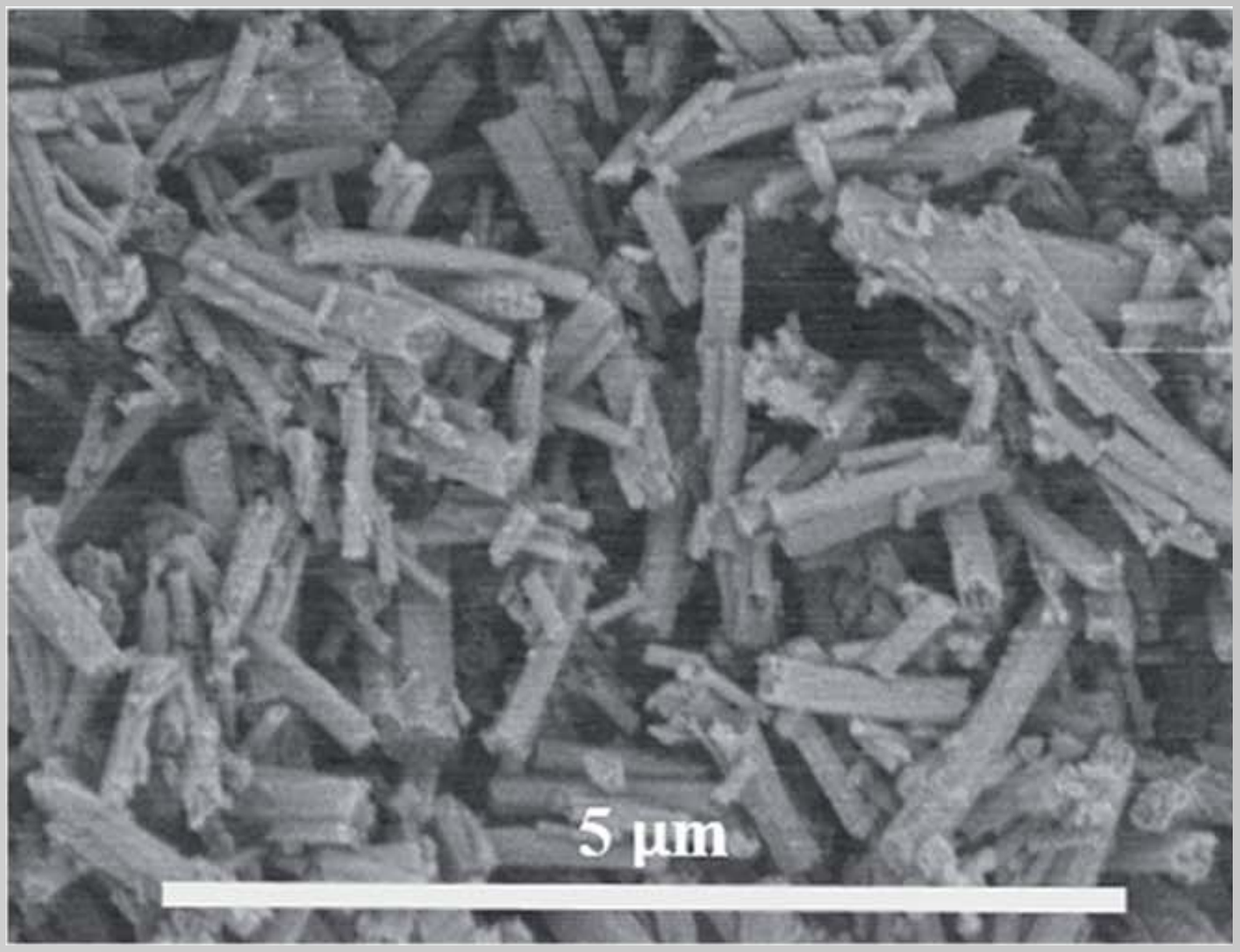


M. Witman, et al Chem. Sci**. 7** (9), 6263 (2016) http://dx.doi.org/10.1039/c6sc01477a

Mg-MOF-74 osalazine





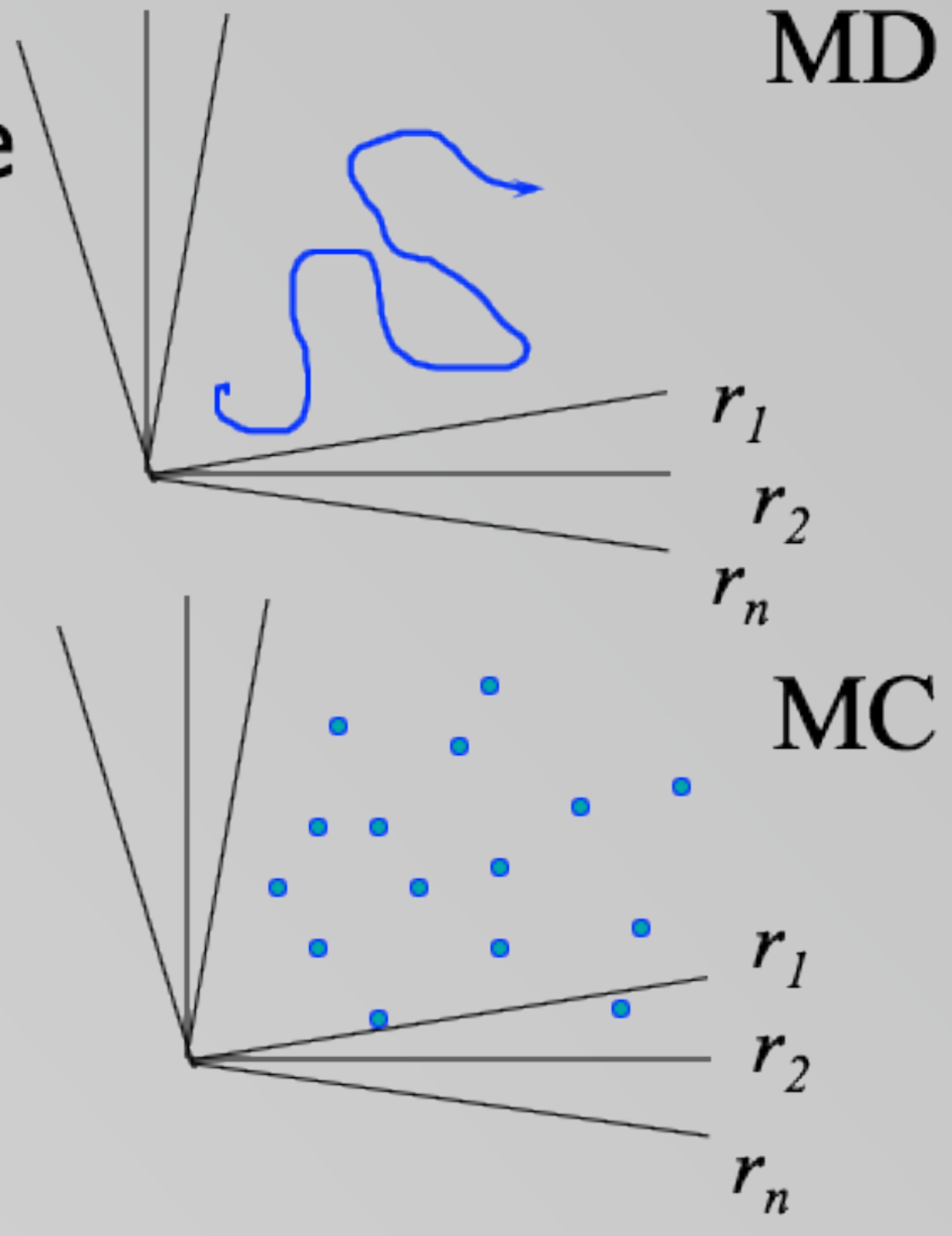


M. Witman, et al Chem. Sci**. 7** (9), 6263 (2016) http://dx.doi.org/10.1039/c6sc01477a

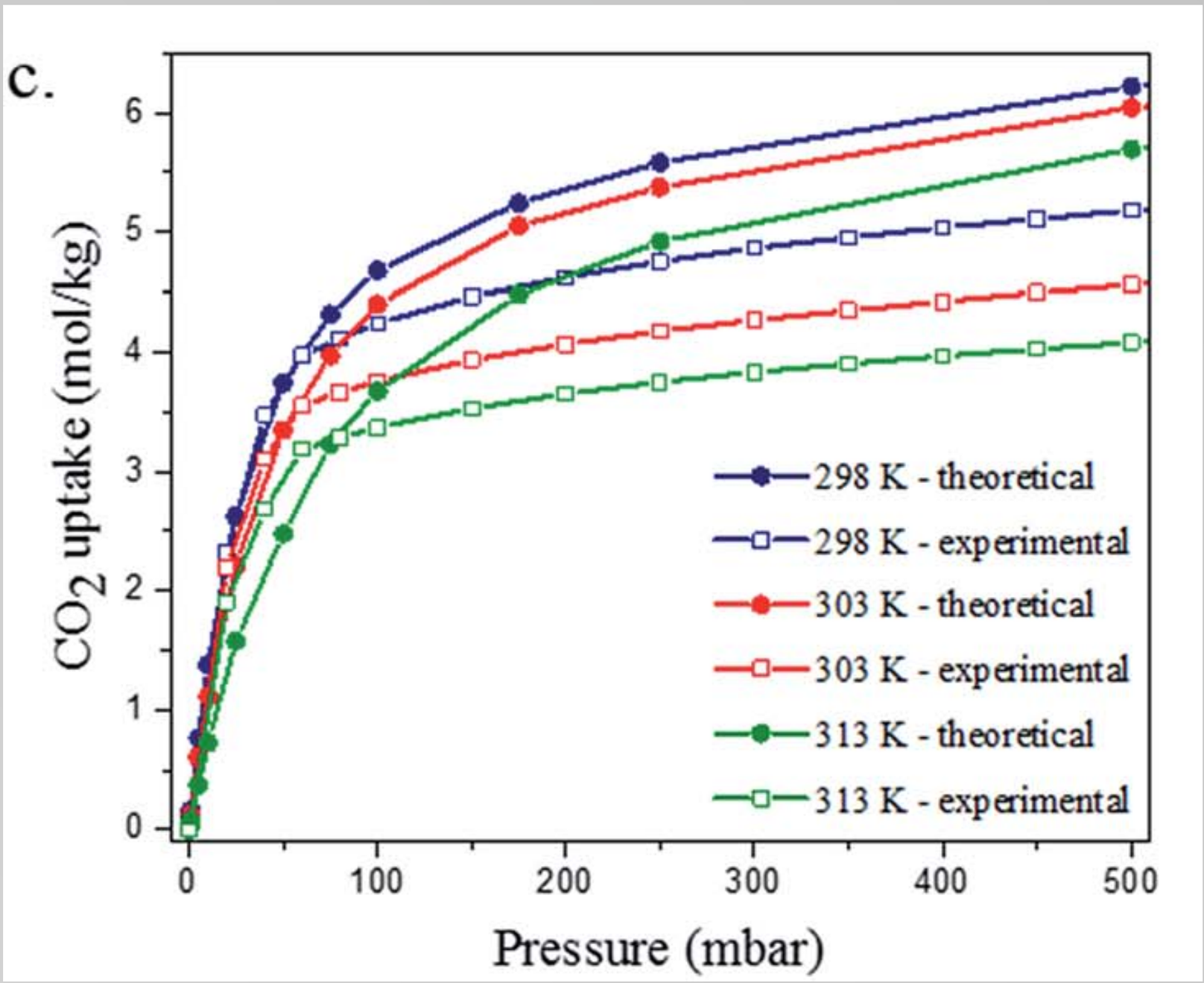
Molecular Simulations

- Molecular dynamics: solve equations of motion
- Monte Carlo: importance sampling

- calculate thermodynamic and transport properties for a given intermolecular potential

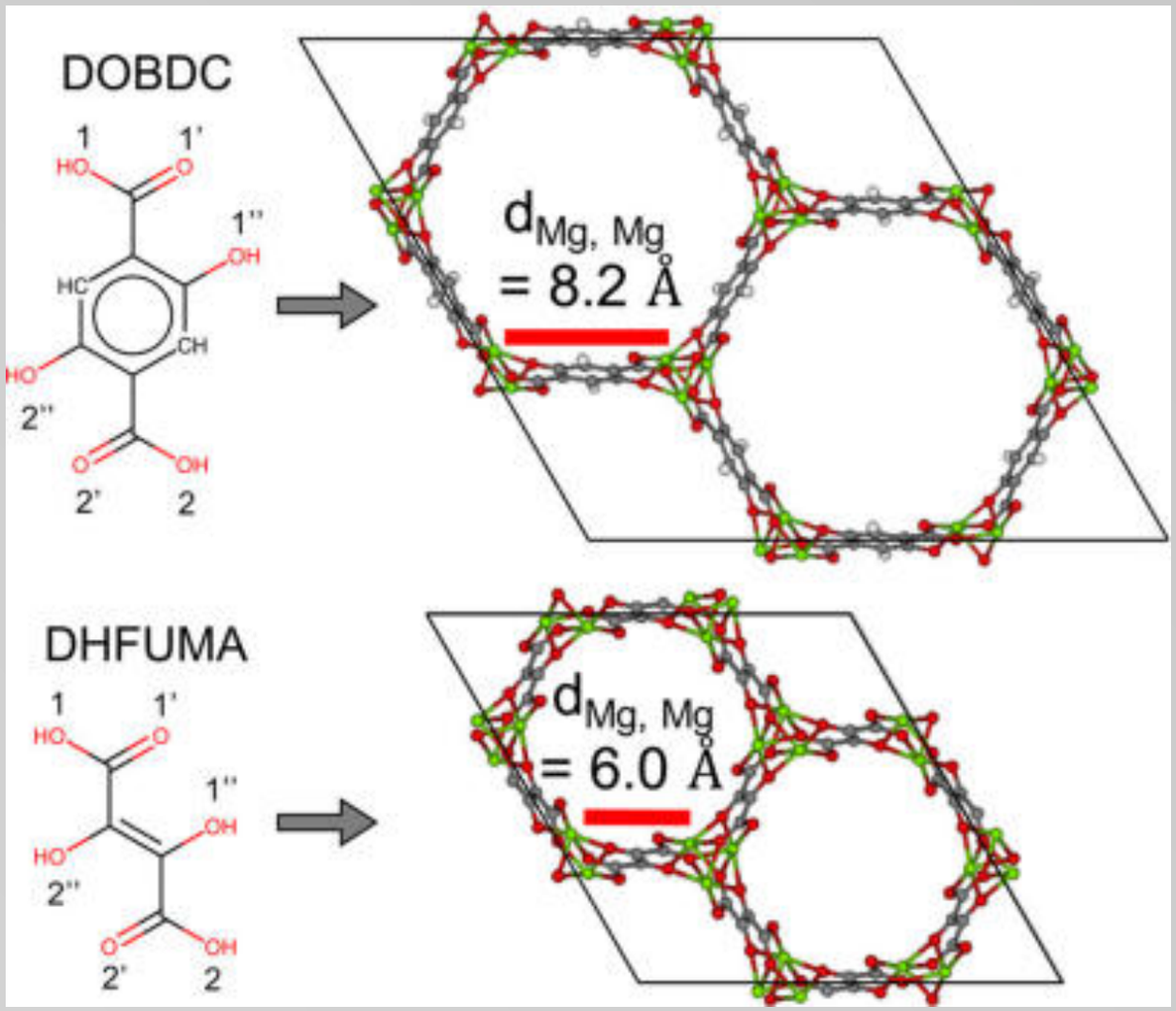


Mg-MOF-74 osalazine



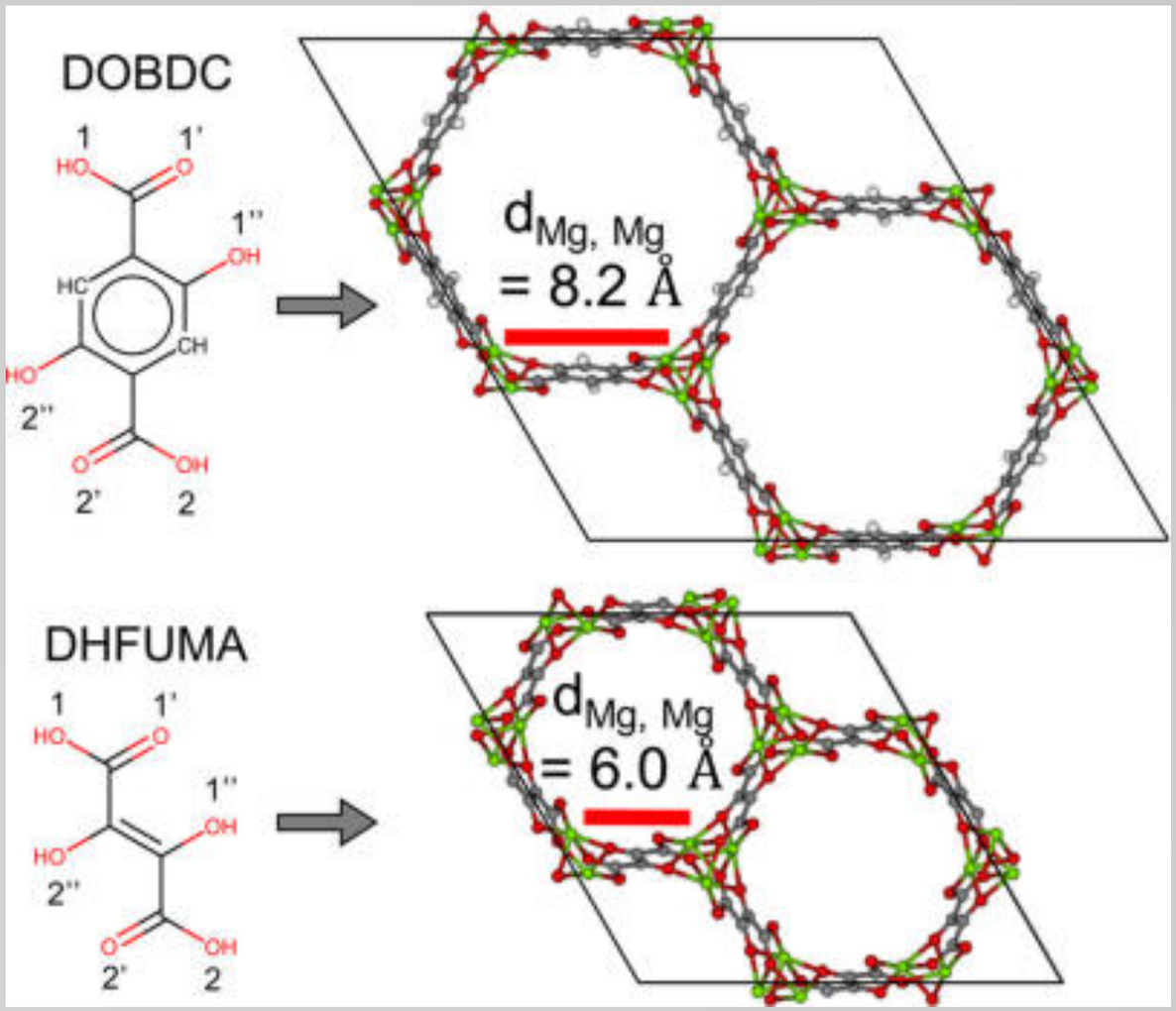
M. Witman, et al Chem. Sci**. 7** (9), 6263 (2016) http://dx.doi.org/10.1039/c6sc01477a

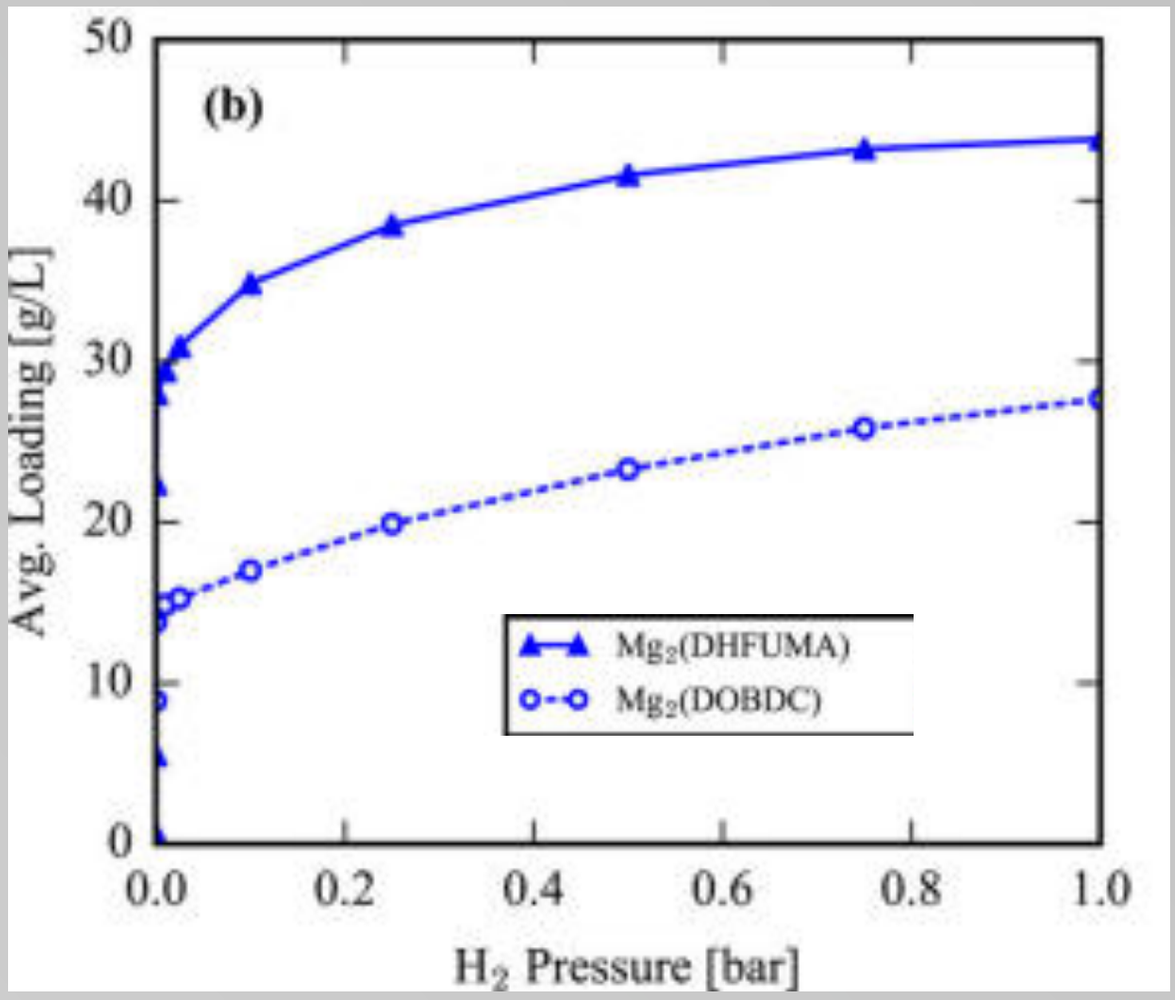
In silico generation of MOF-74 analogs: record hydrogen storage



M. Witman *et al*, J Phys Chem C 121 (2), 1171 (2017)

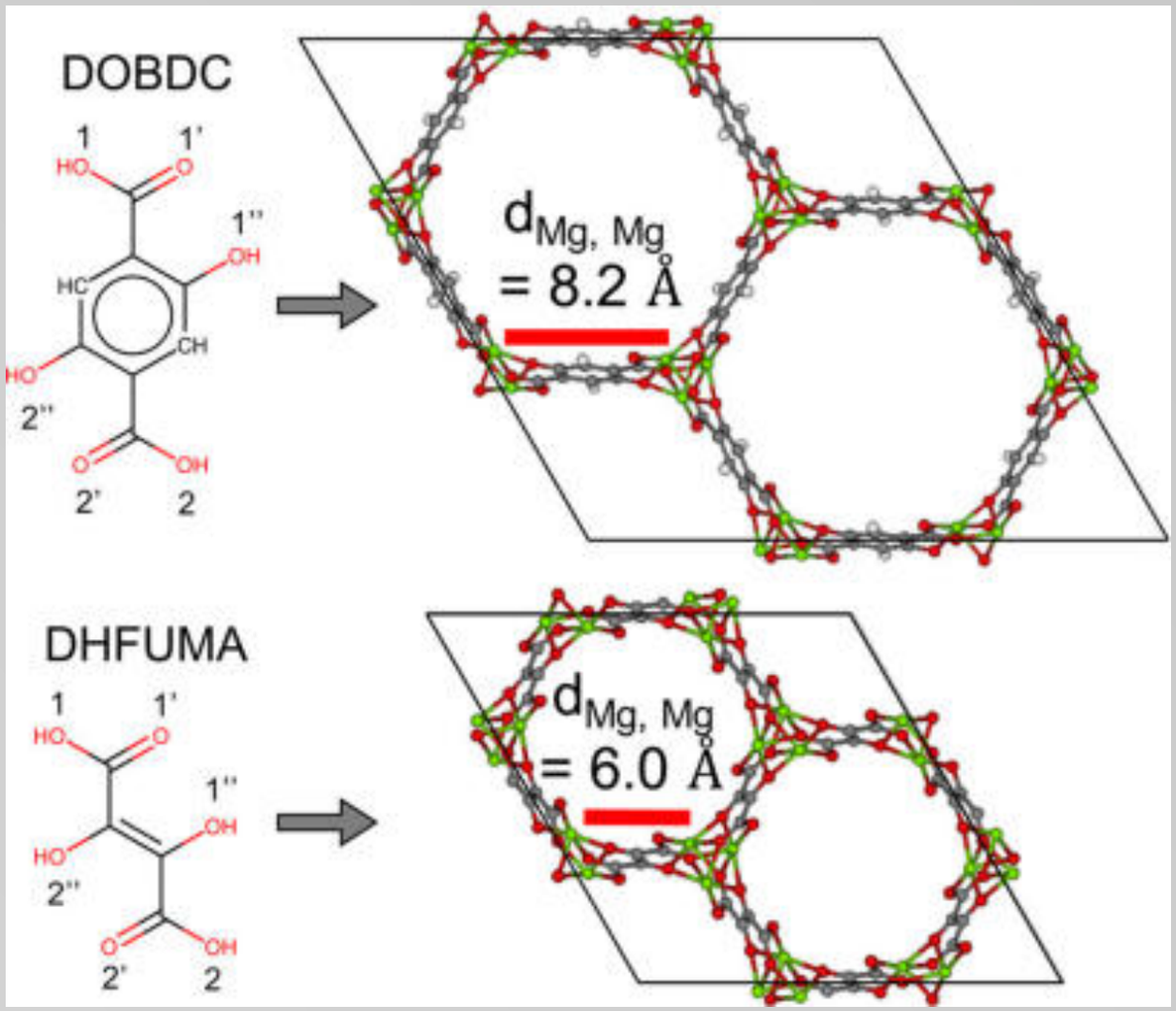
In silico generation of MOF-74 analogs: record hydrogen storage

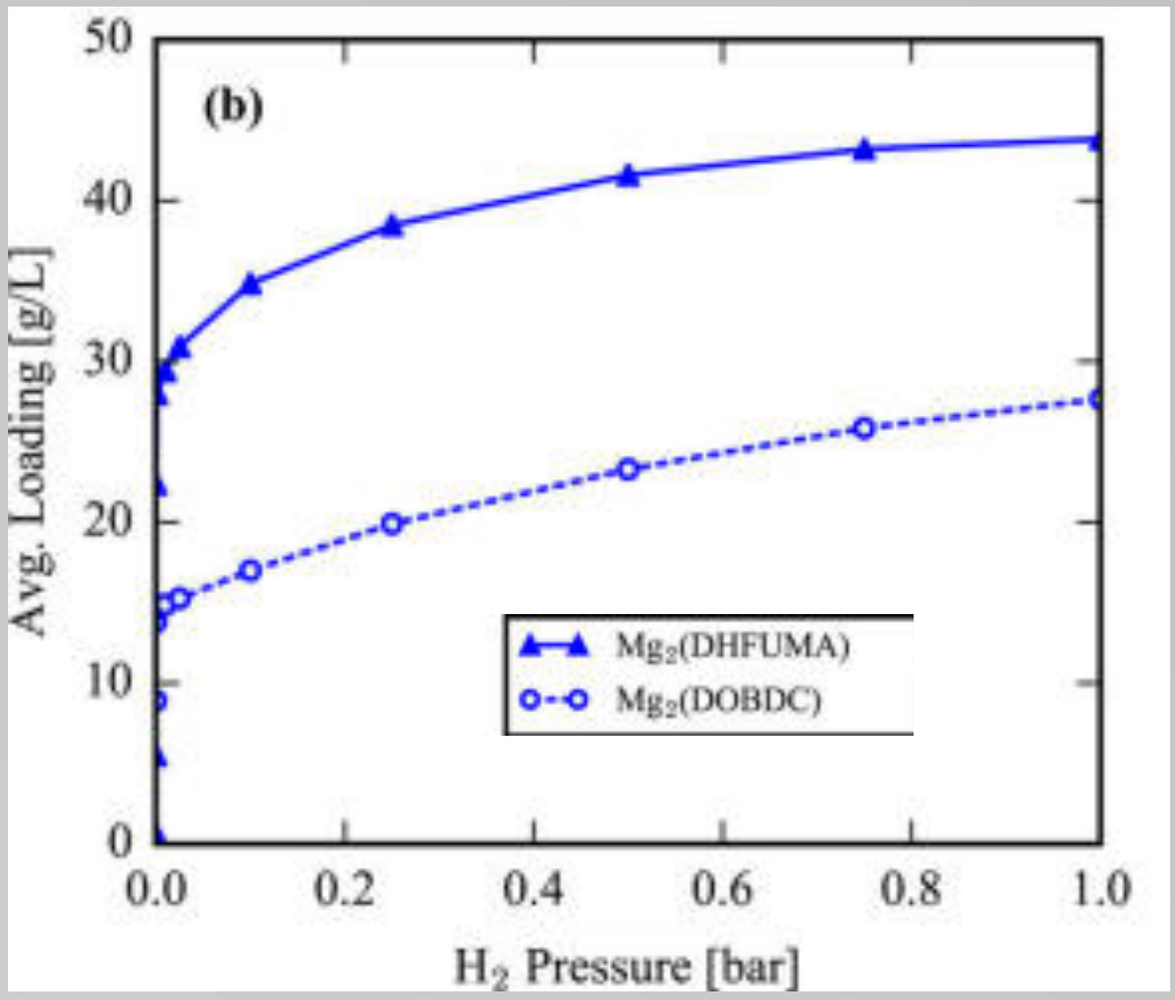




M. Witman *et al*, J Phys Chem C 121 (2), 1171 (2017)

In silico generation of MOF-74 analogs: record hydrogen storage





Material can be synthesized (Omar, Northwestern) but not activated

M. Witman *et al*, J Phys Chem C 121 (2), 1171 (2017)

Xe/Kr separations

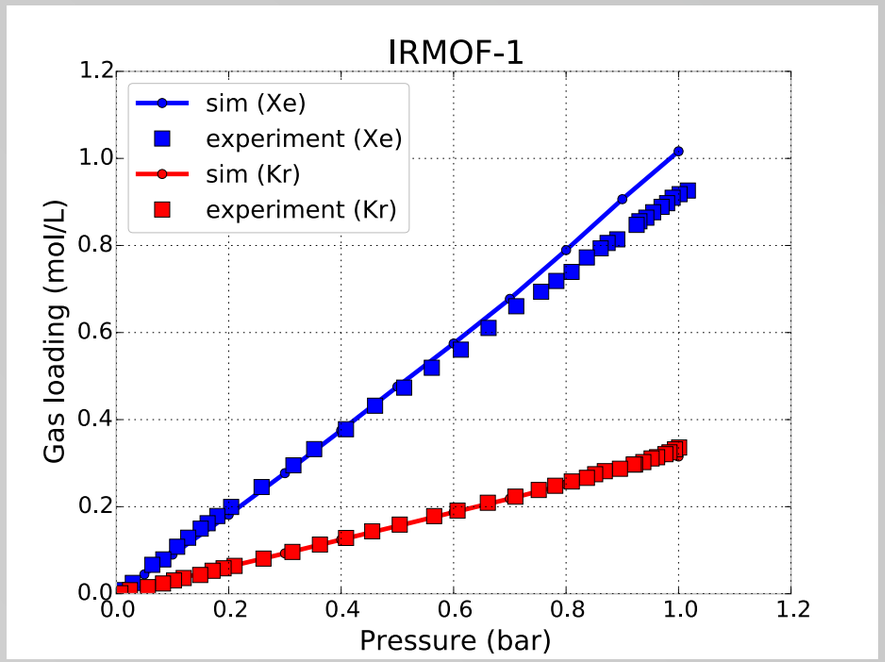
Separations of Xe/Kr

- Nuclear energy reprocessing: Xe - Kr isotopes are produced (i.e., ^{85}Kr with $t_{1/2}$ = 10.8 y)
- Xe used in several applications : cryogenic distillation of air:
  - pure Xe $5000 kg

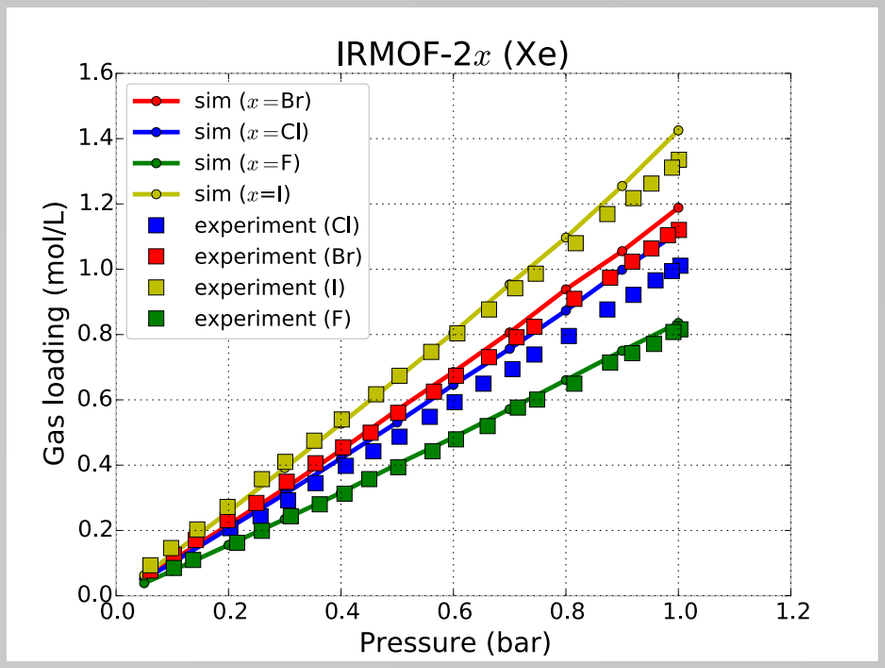
D. Banerjee, C. M. Simon, A. M. Plonka, R. K. Motkuri, J. Liu, X. Chen, B. Smit, J. B. Parise, M. Haranczyk, and P. K. Thallapally, *Metal-organic framework with optimally selective xenon adsorption and separation* Nat. Comm. **7** (11831) (2016) http://dx.doi.org/10.1038/ncomms11831

C. M. Simon, R. Mercado, S. K. Schnell, B. Smit, and M. Haranczyk, *What Are the Best Materials To Separate a Xenon/Krypton Mixture?* Chem. Mat. **27** (12), 4459 (2015) http://dx.doi.org/10.1021/acs.chemmater.5b01475

Comparison with experimental data



(a)



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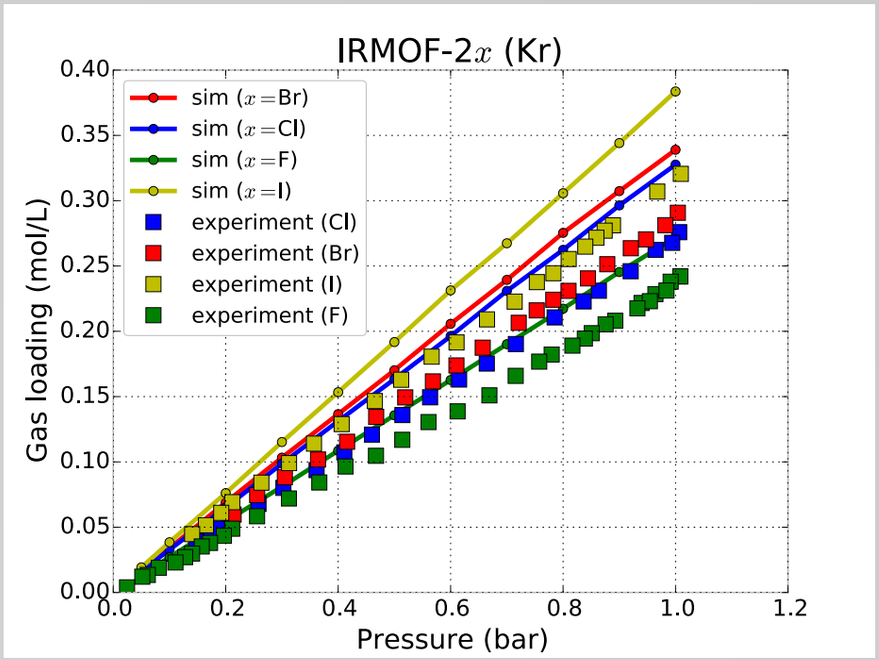
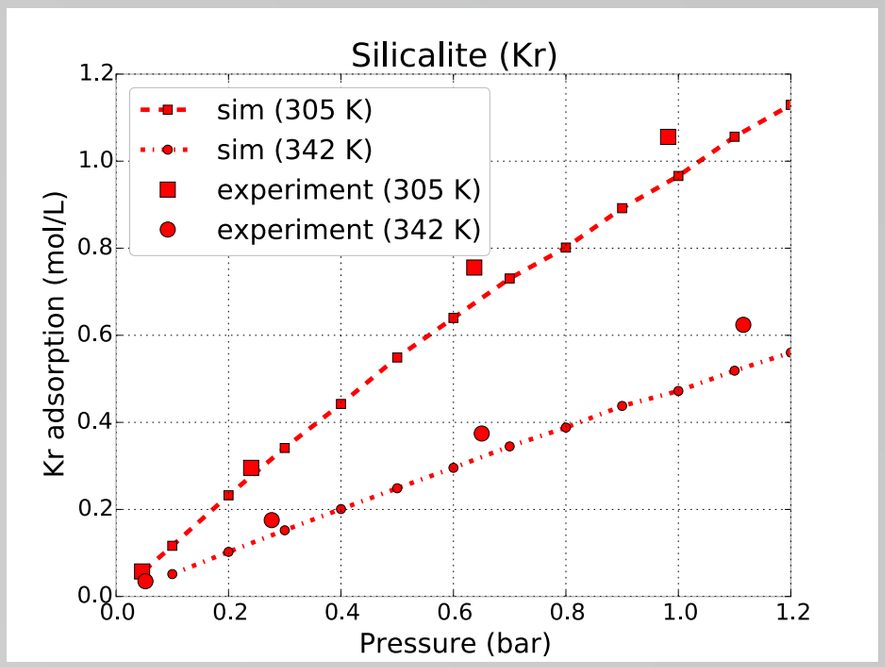


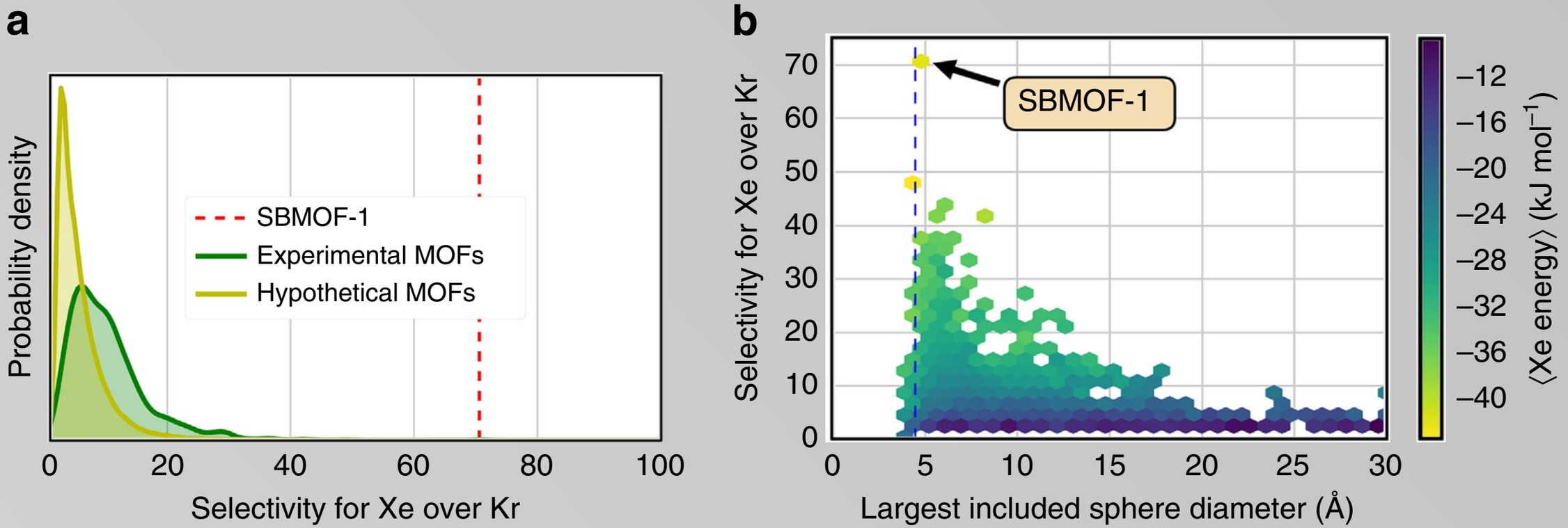
(c)



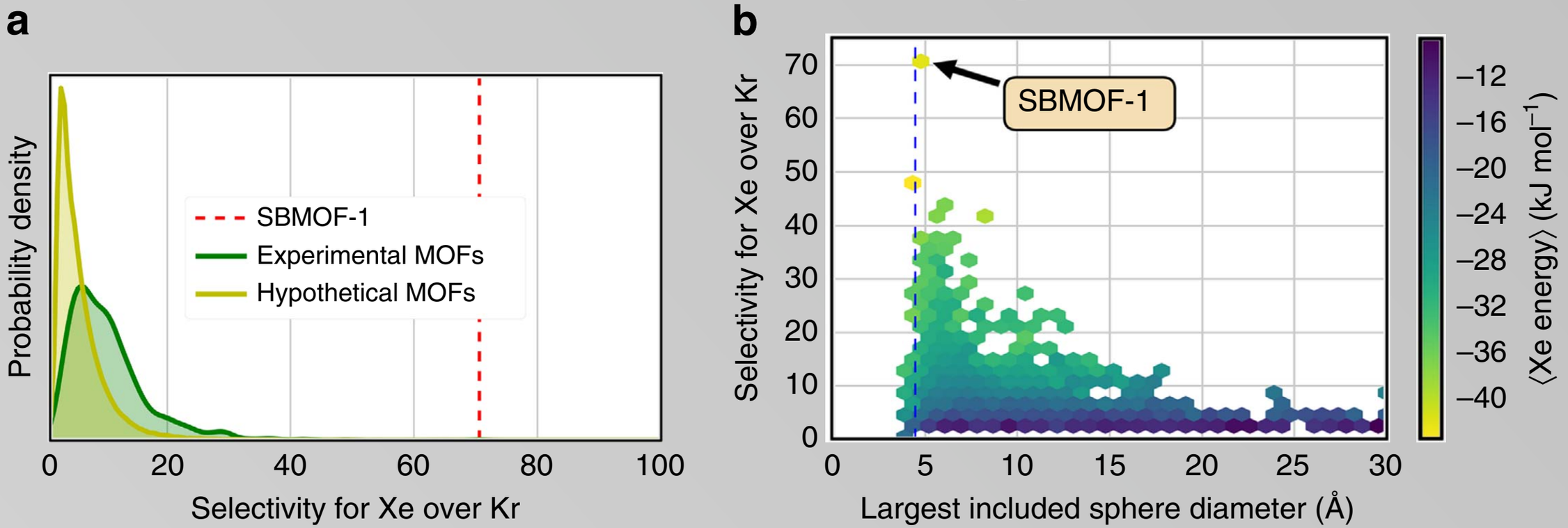
(d)

C. M. Simon, R. Mercado, S. K. Schnell, B. Smit, and M. Haranczyk, *What Are the Best Materials To Separate a Xenon/ Krypton Mixture?* Chem. Mat. **27** (12), 4459 (2015) http://dx.doi.org/10.1021/acs.chemmater.5b01475

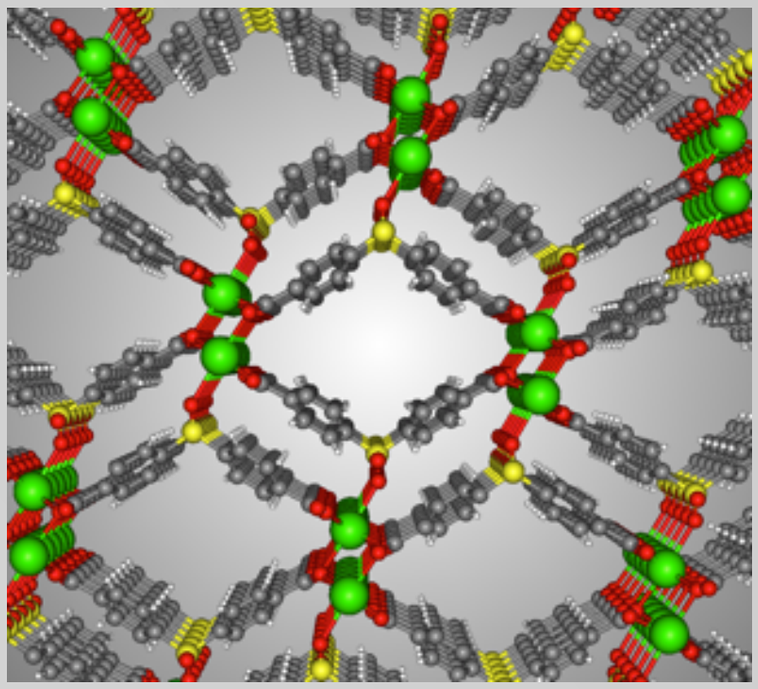
Screening

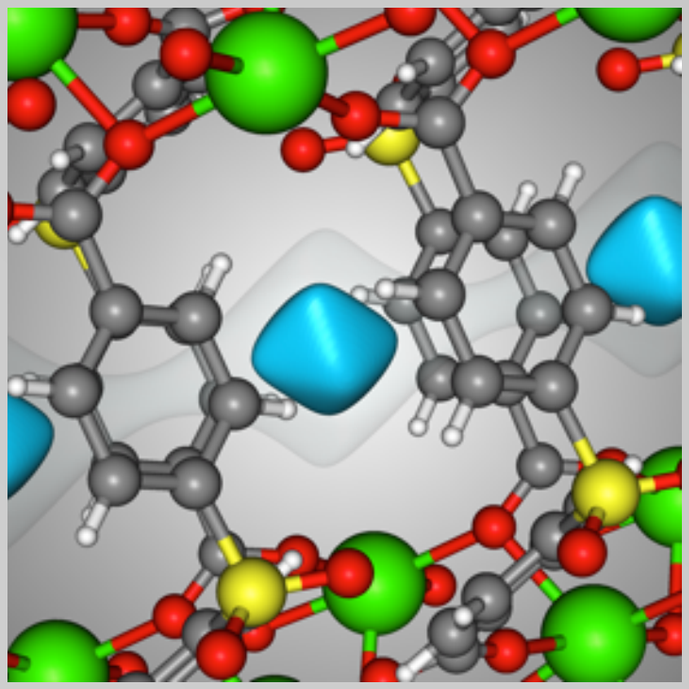

a
Probability density
SBMOF-1
Experimental MOFs
Hypothetical MOFs
0
20
40
60
80
100
Selectivity for Xe over Kr
b
Selectivity for Xe over Kr
70
60
50
40
30
20
10
0
SBMOF-1
0
5
10
15
20
25
30
Largest included sphere diameter (Å)
−12
−16
−20
−24
−28
−32
−36
−40
⟨Xe energy⟩ (kJ mol−1)

Screening

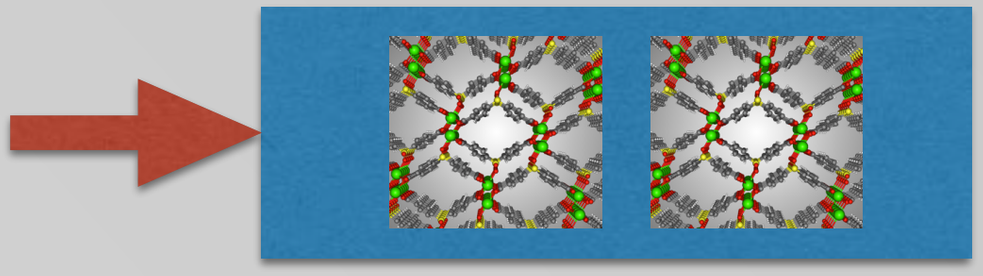


Top performing: SBMOF-1





Experiments: SBMOF-1



Model Mixture:

O_2, N_2, CO_2, Kr, Xe

(400 ppm Xe, 40 ppm Kr,
78.1% N_2, 20.9% O_2,
0.03% CO_2, and 0.9% Ar)

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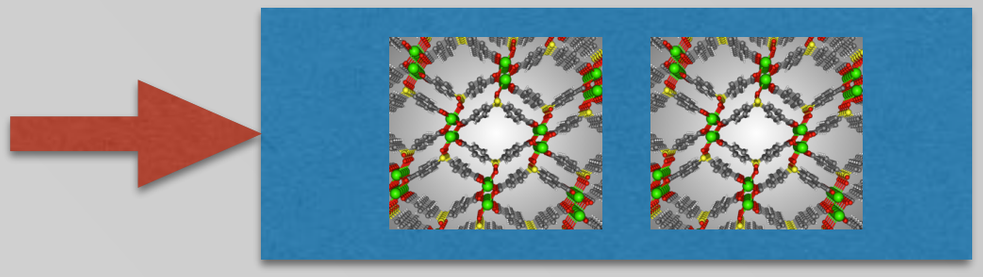

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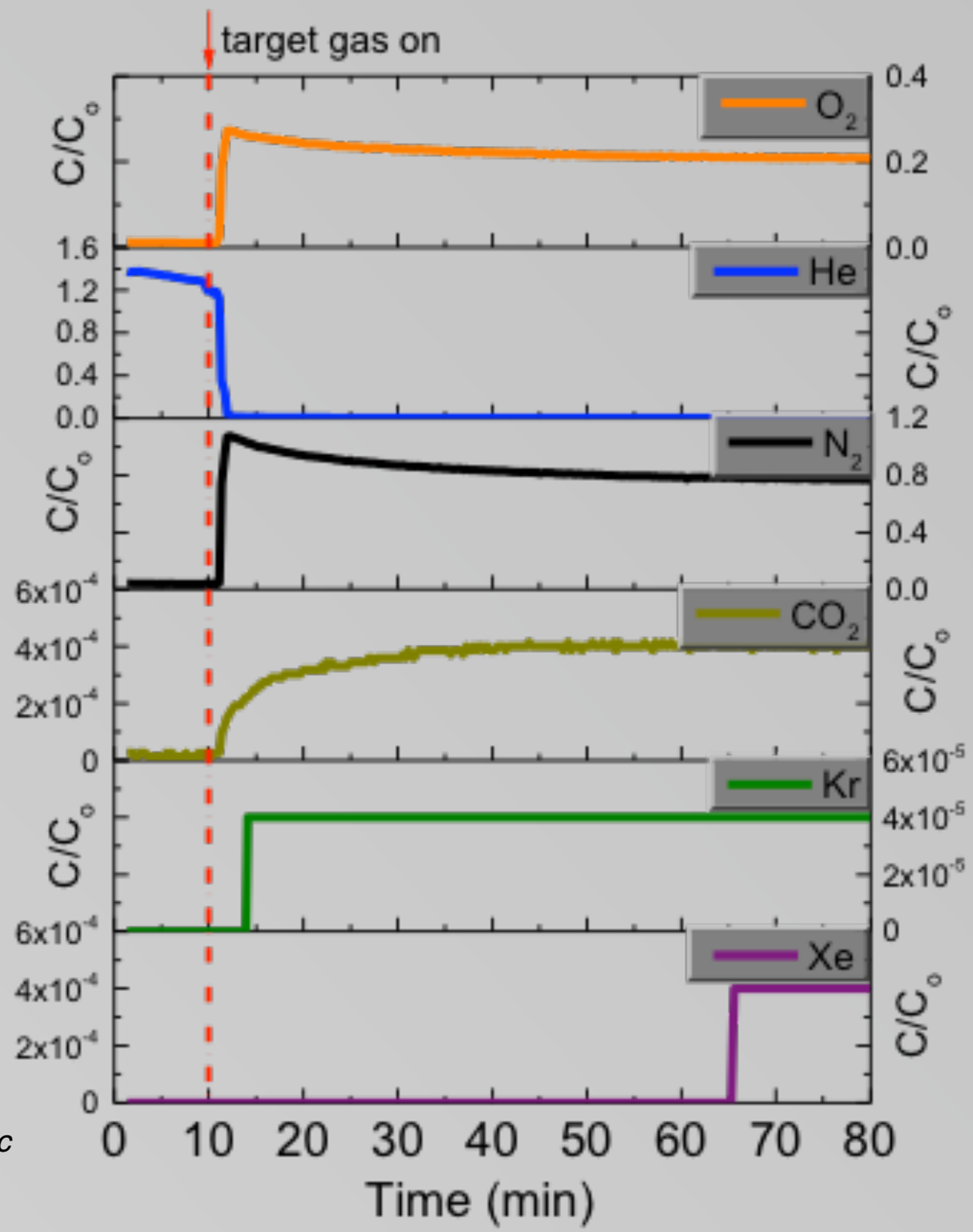

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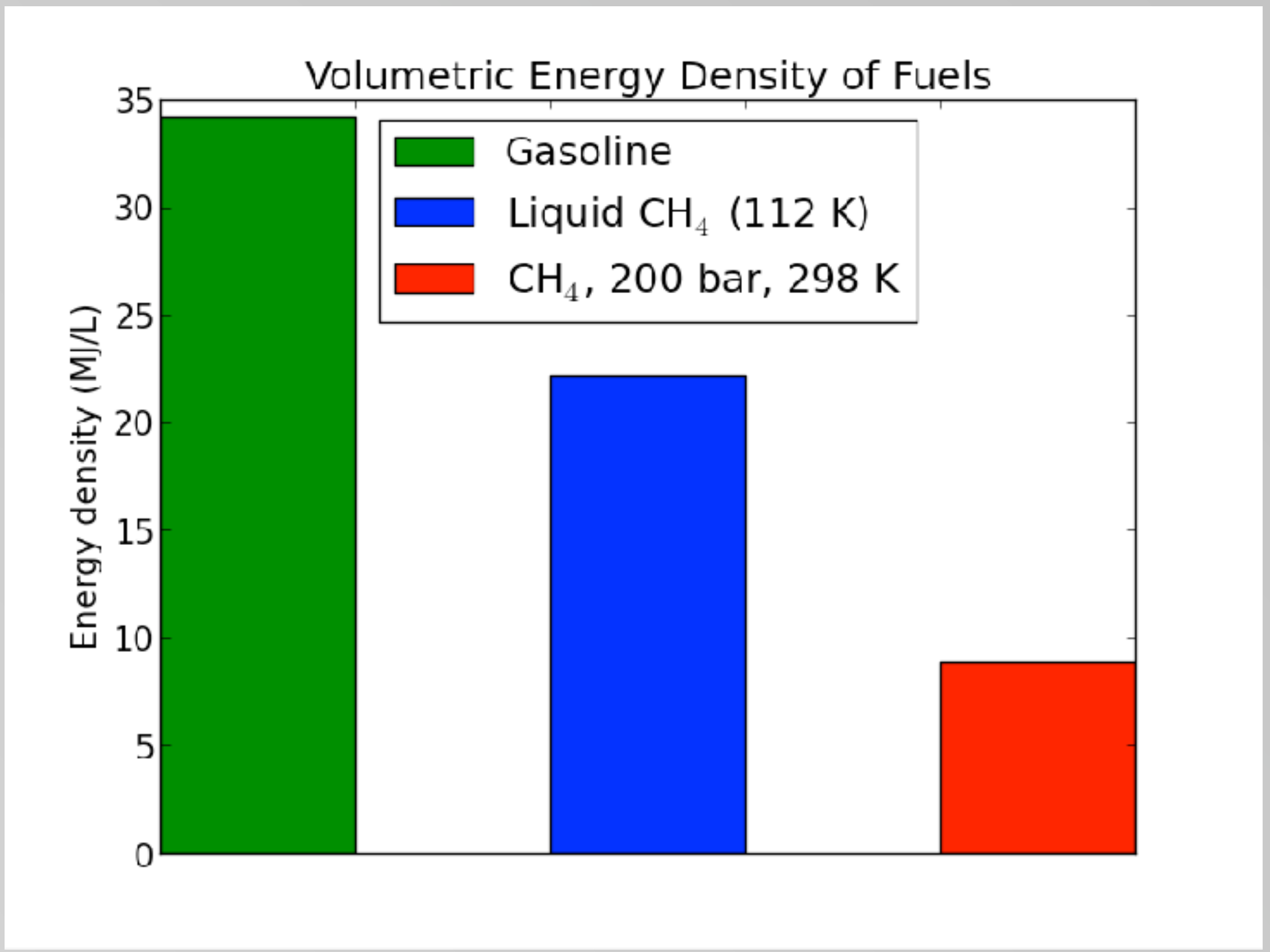
Methane Storage

Methane in cars: energy density

0.036 MJ

34.2 MJ

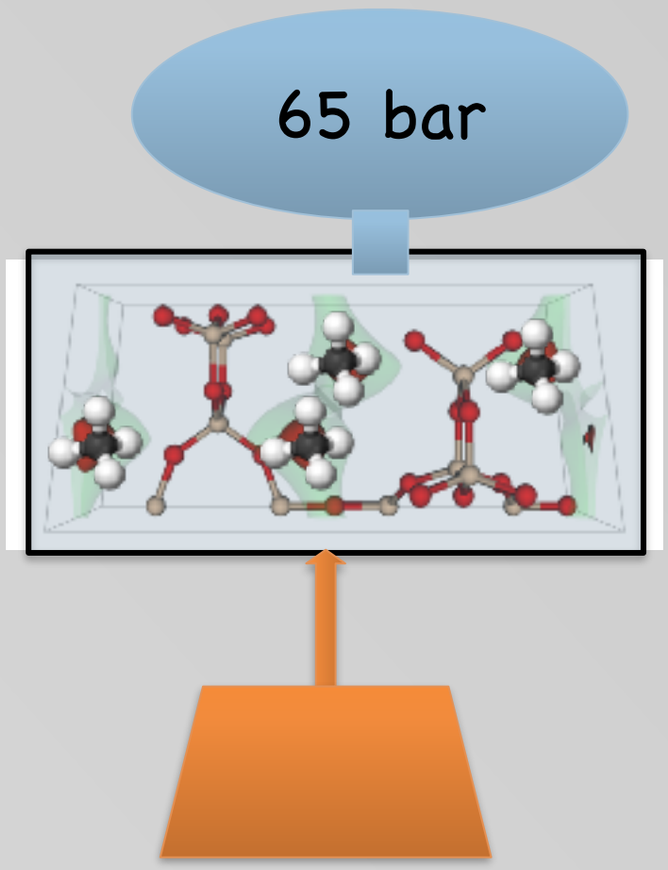
Methane versus gasoline



Makal *et a*l. *Chem. Soc. Rev.* **2012** 41.23, 7761-7779.

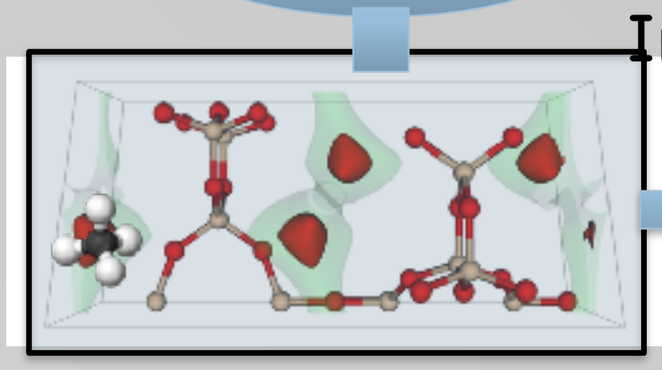
Nano porous materials?

65 bar



P_H = 65 bar

5.8 bar



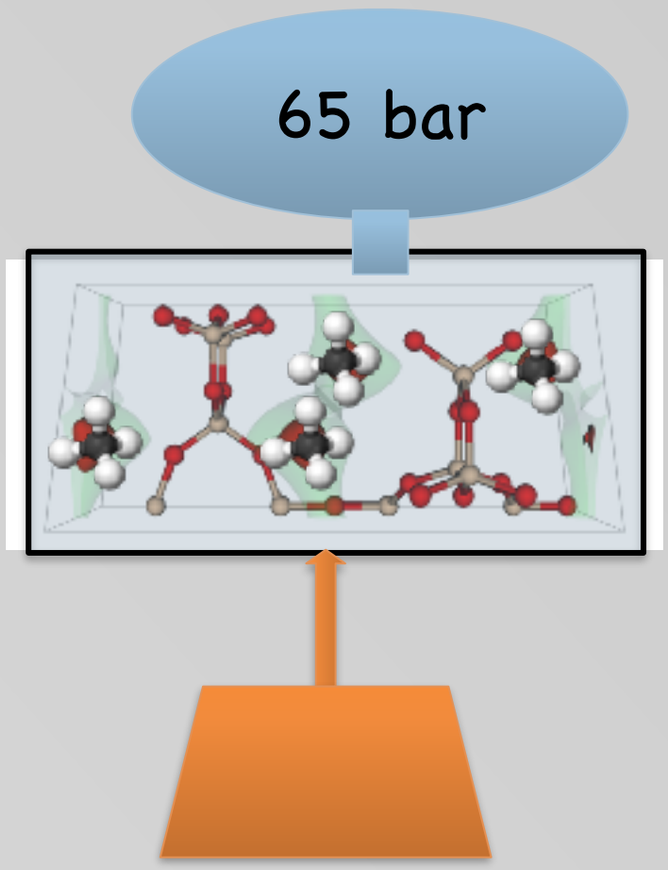
Insufficient flow

~1 bar

P_L = 5.8 bar

Can we find a material with the same energy density as compressed natural gas?

65 bar



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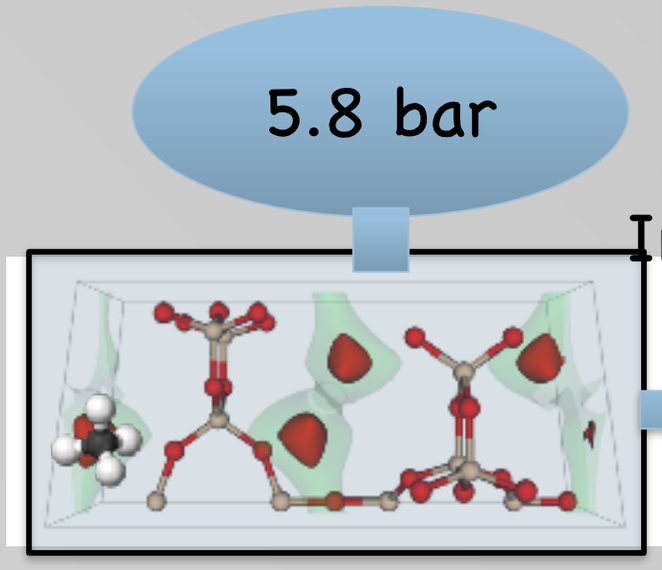
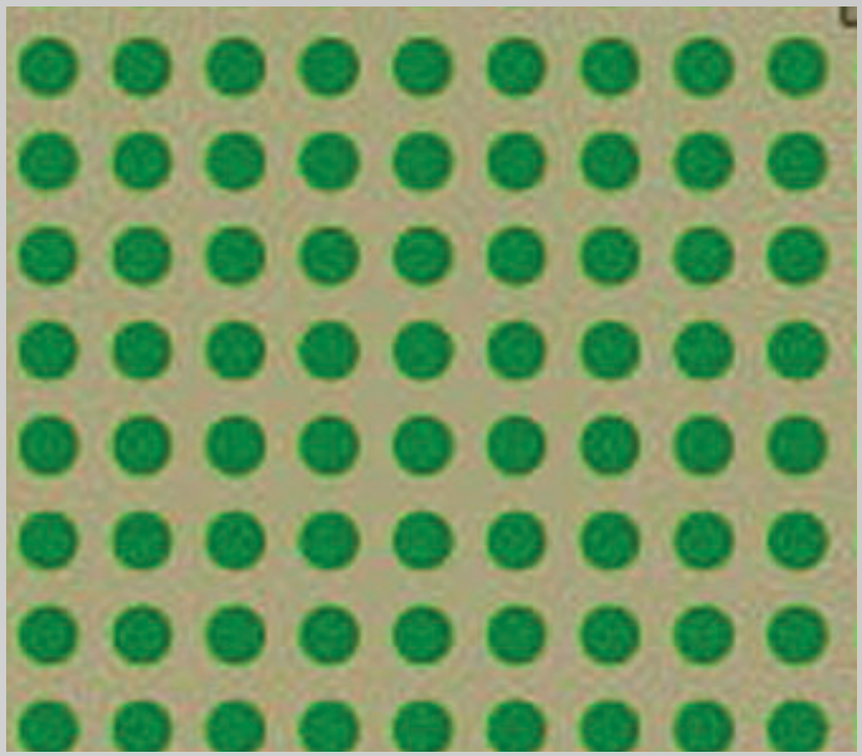


Insufficient flow

~1 bar

P_L = 5.8 bar

What is the best material?



Langmuir isotherm:

$$\sigma = \frac{\beta\varepsilon e^{-\beta U_0} P}{1 + \frac{\beta\varepsilon e^{-\beta U_0}}{M} P},$$

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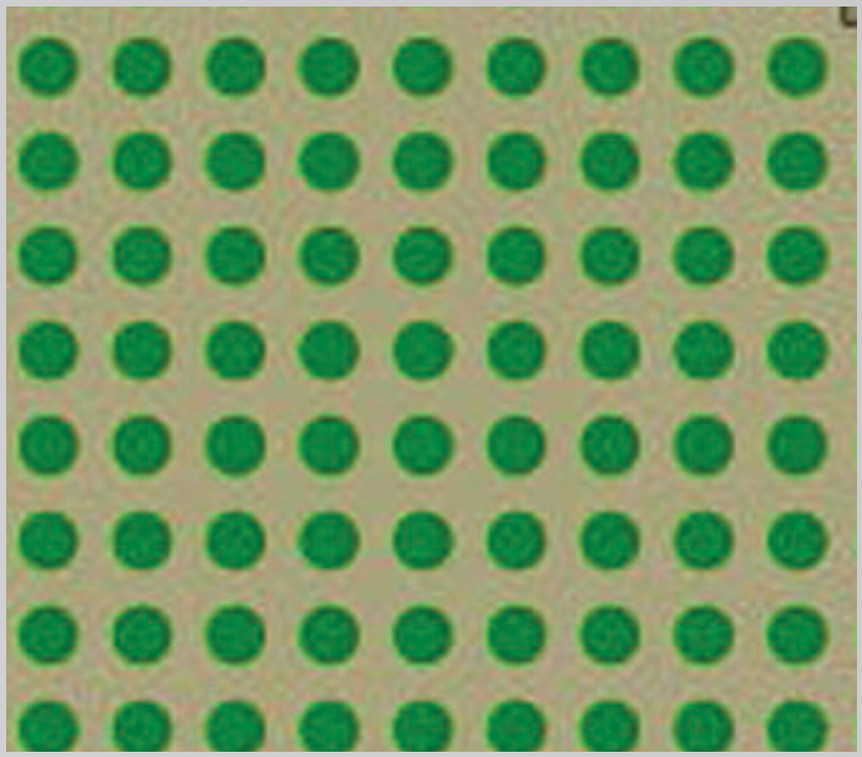

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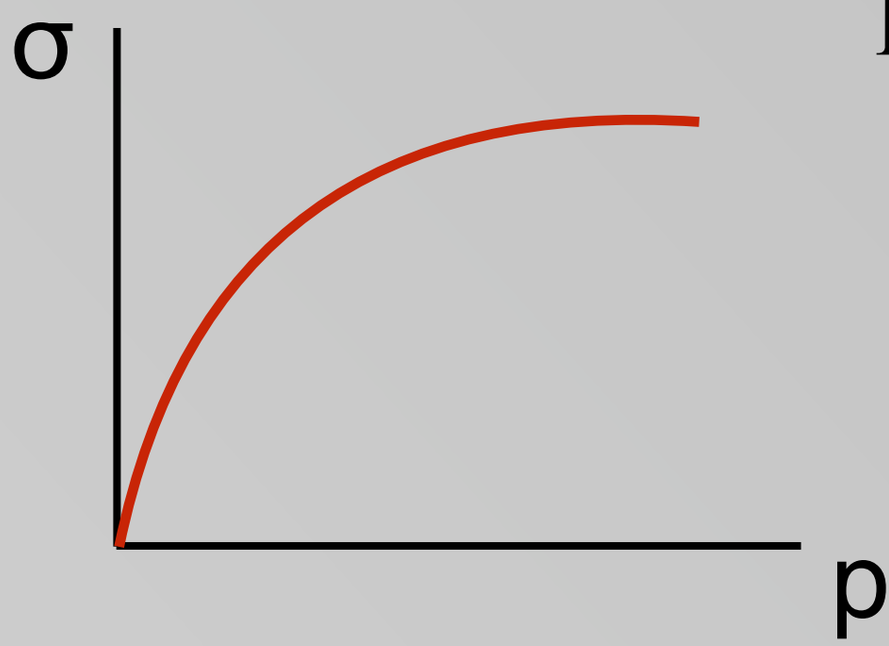

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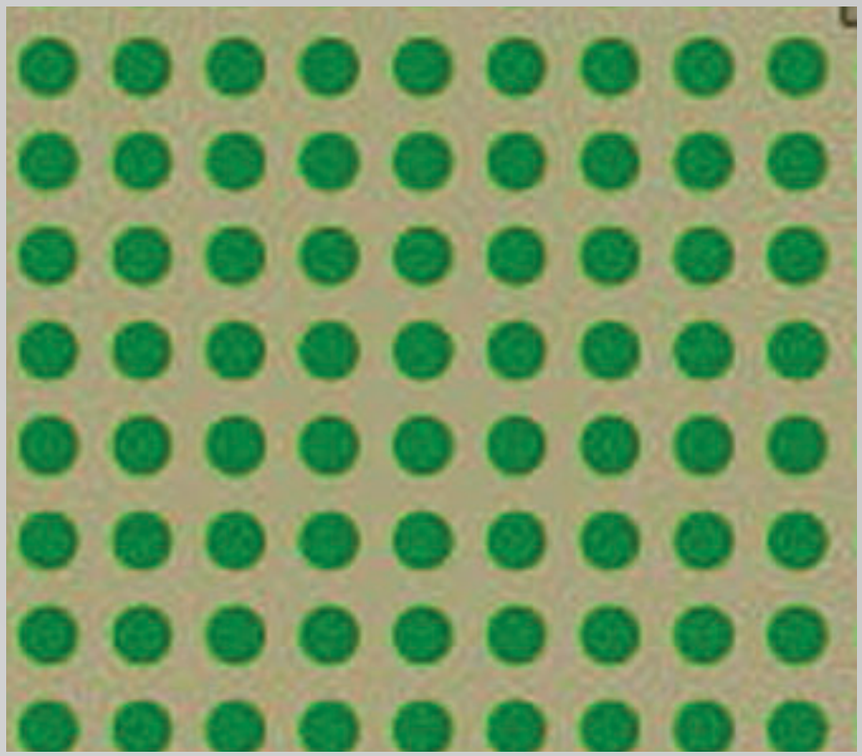

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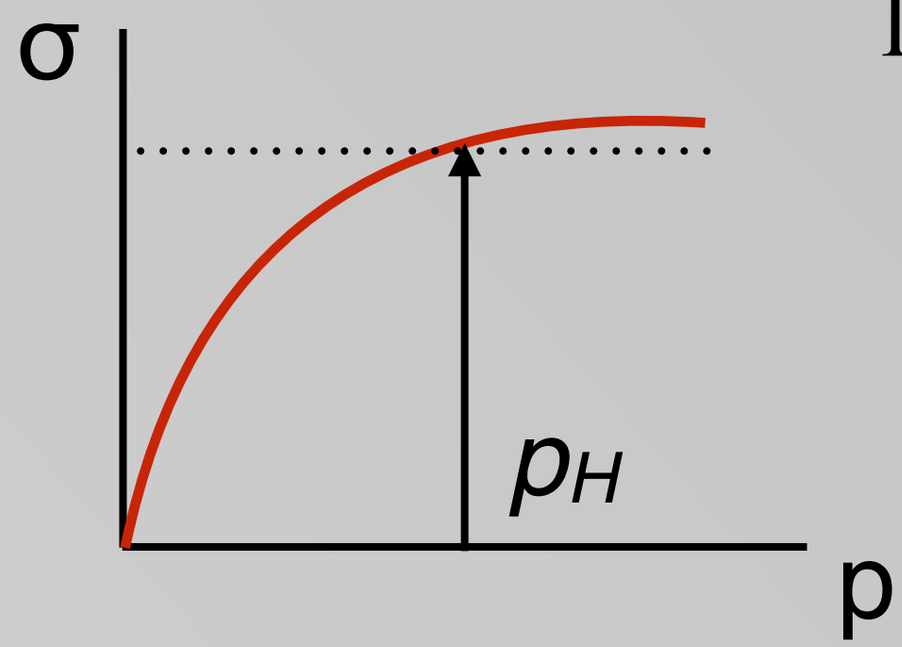

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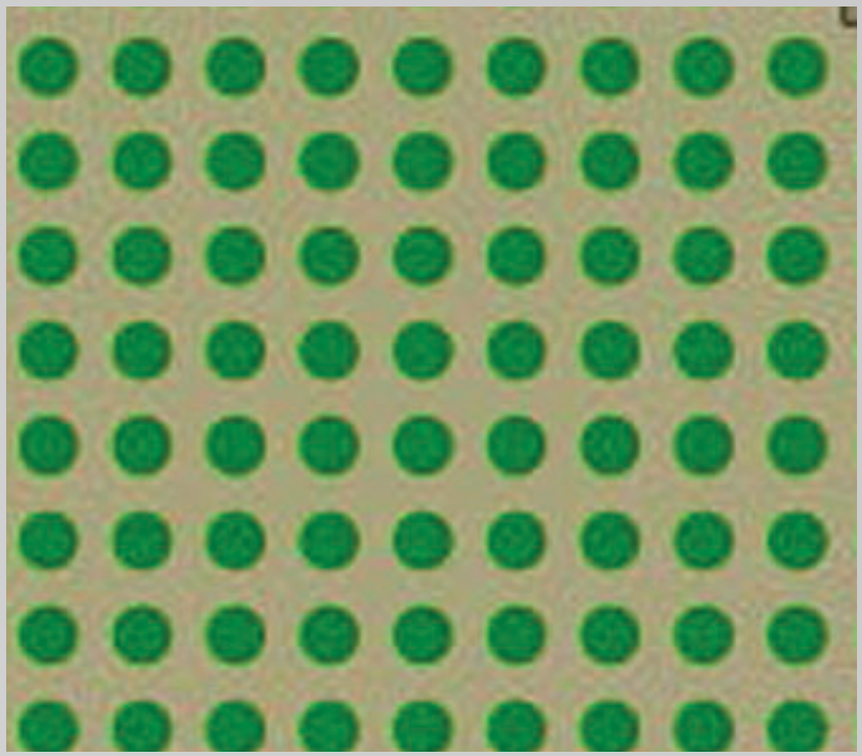

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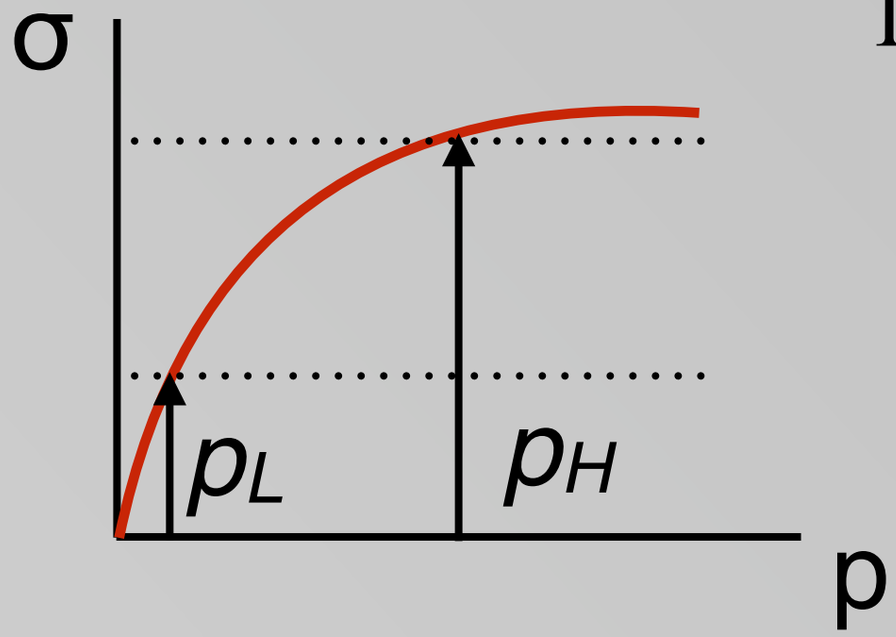

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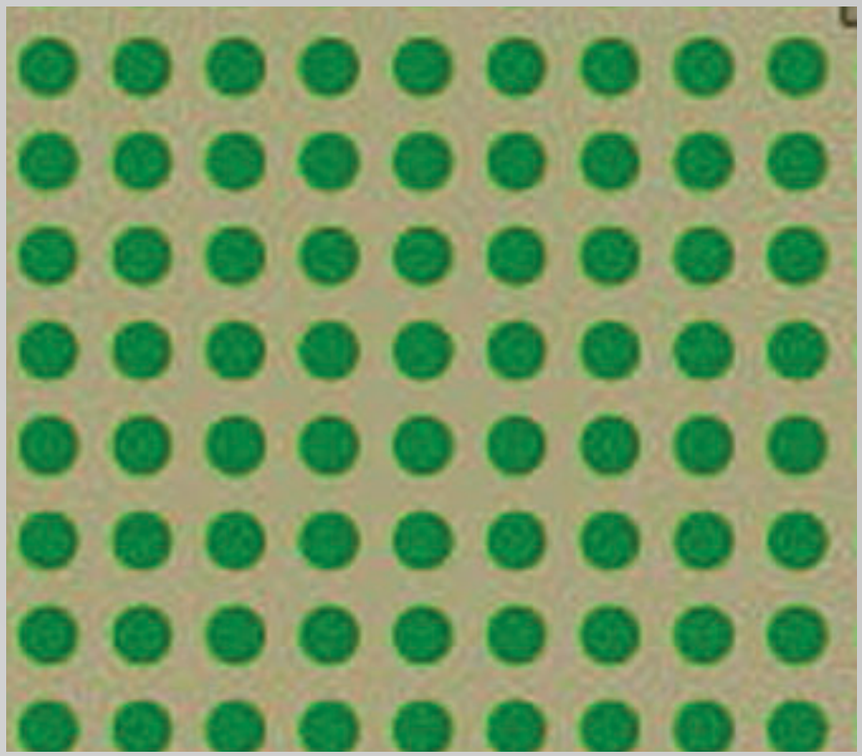

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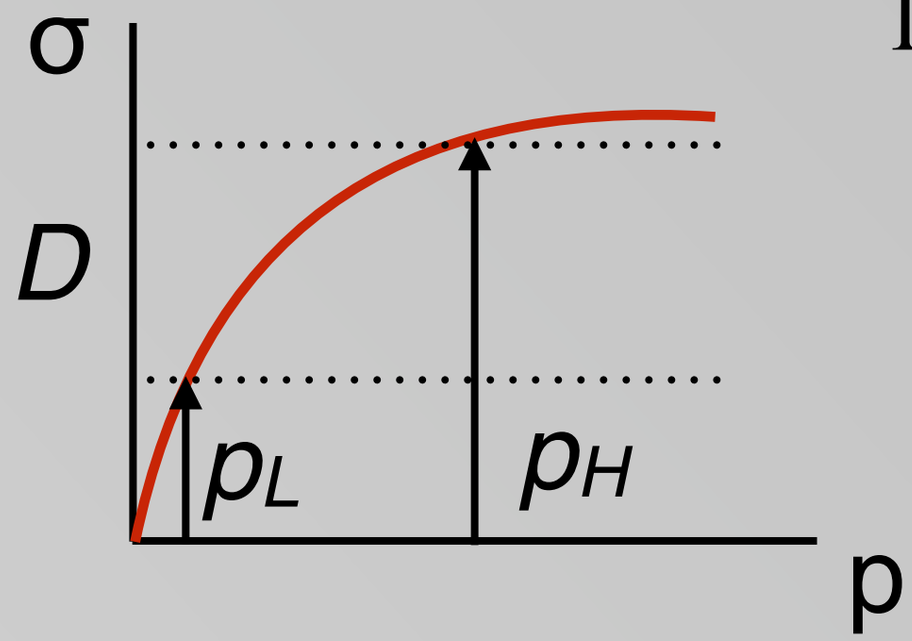

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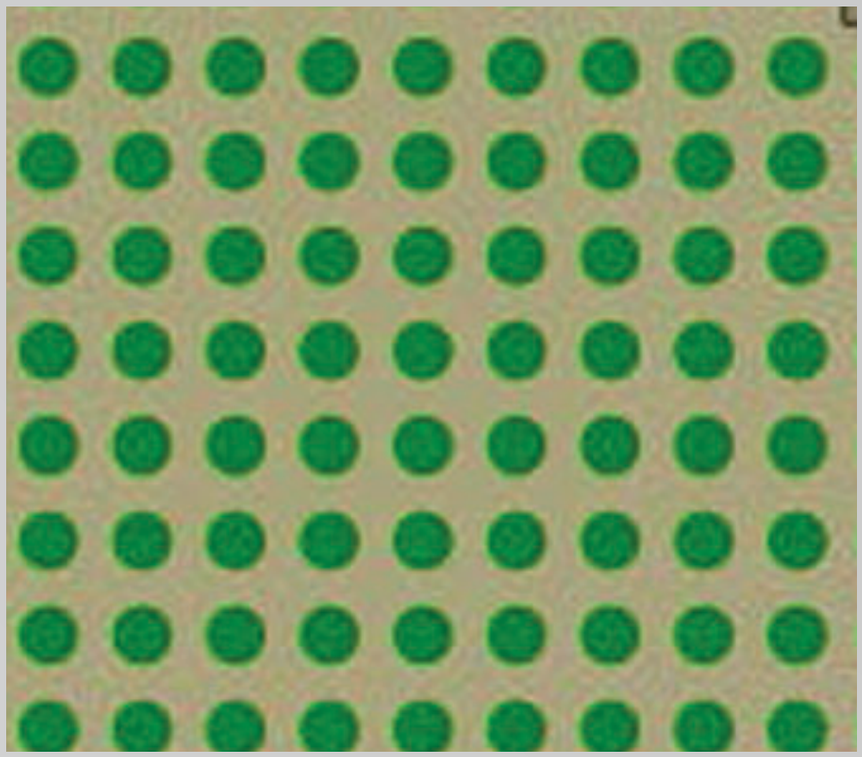

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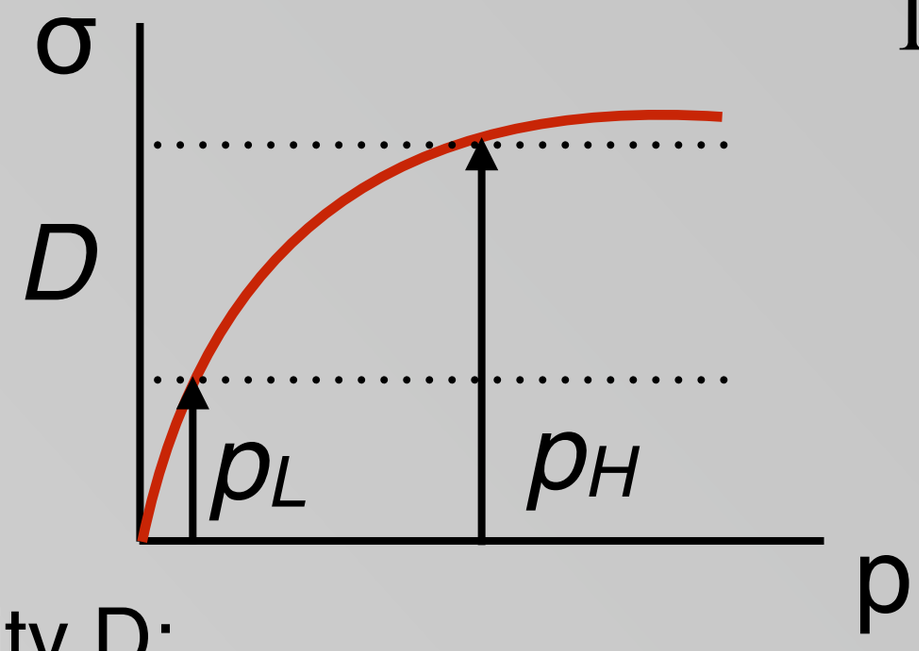

Fractional deliverable capacity D:

$$D(U_0; P_{\mathrm{L}}, P_{\mathrm{H}}) = \frac{\beta\varepsilon e^{-\beta U_0} P_{\mathrm{H}}}{1 + \frac{\beta\varepsilon e^{-\beta U_0}}{M} P_{\mathrm{H}}} - \frac{\beta\varepsilon e^{-\beta U_0} P_{\mathrm{L}}}{1 + \frac{\beta\varepsilon e^{-\beta U_0}}{M} P_{\mathrm{L}}},$$

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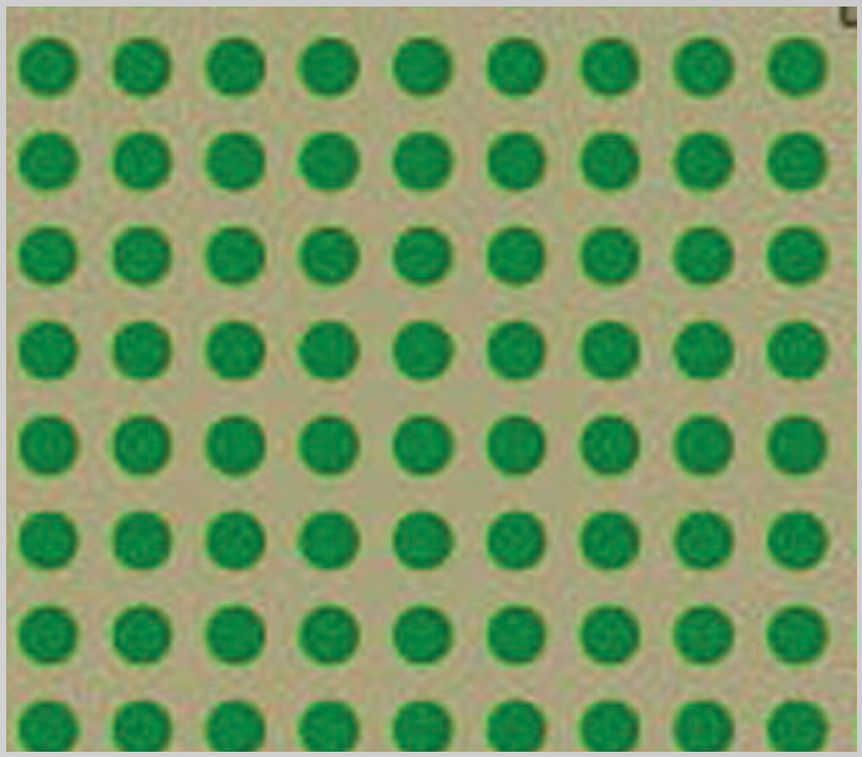

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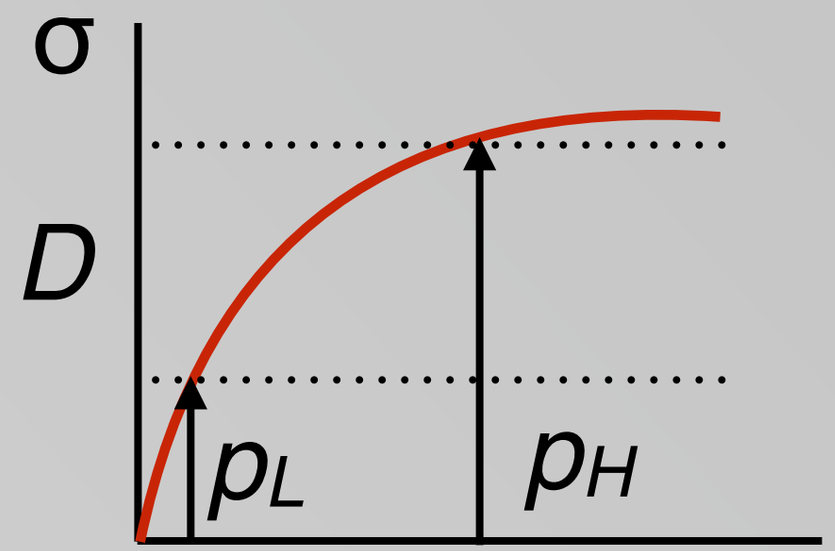

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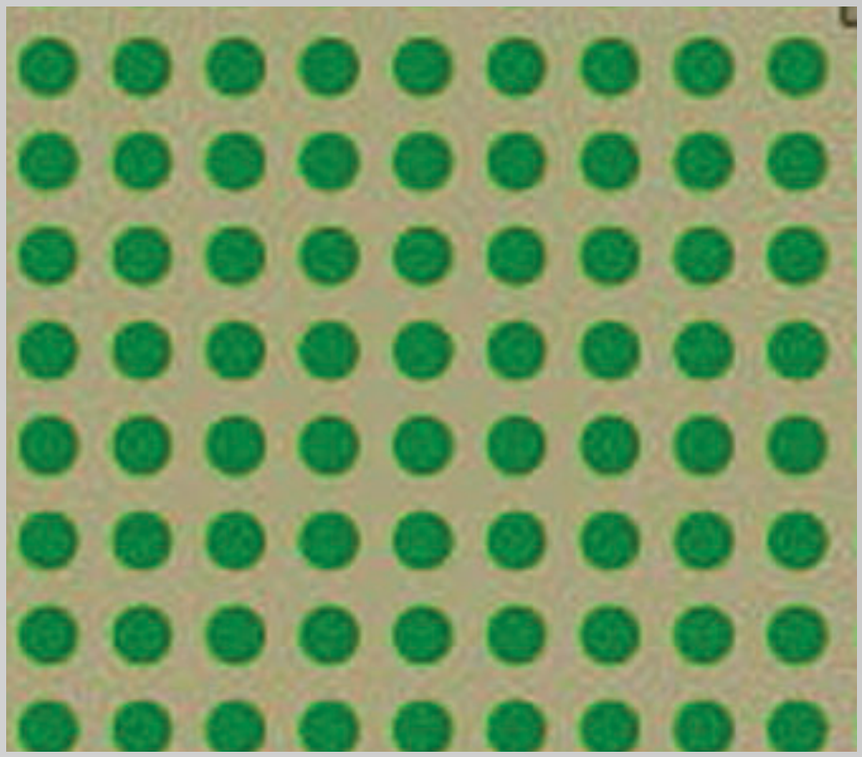
Optimal energy

$$U_{0,\mathrm{opt}} = U_{0,\mathrm{opt}}\left(\frac{\varepsilon}{M}\right) = RT \ln\left(\frac{\sqrt{P_\mathrm{L} P_\mathrm{H}}}{RT} \frac{\varepsilon}{M}\right).$$

What is the best material?



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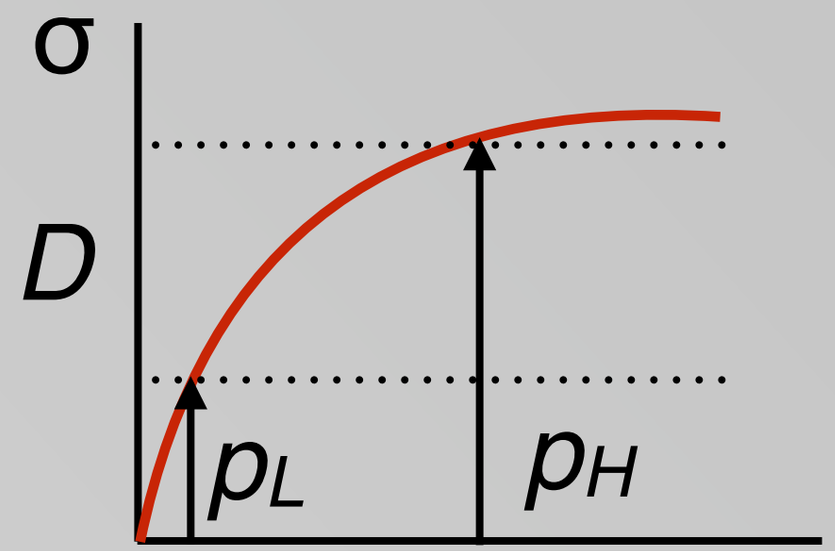

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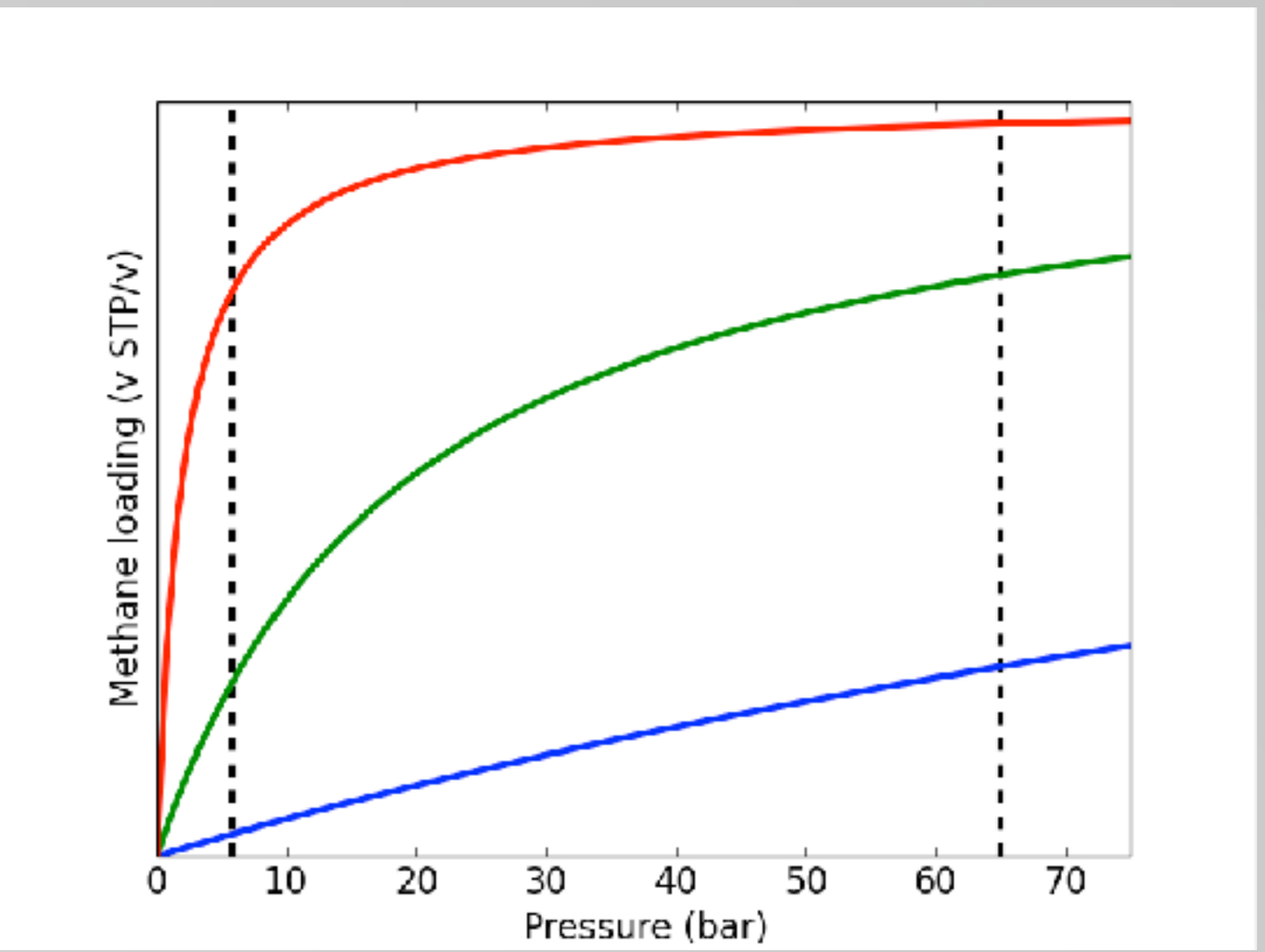
As many adsorption sites as possible with the optimal energy

Goal: maximize deliverable capacity



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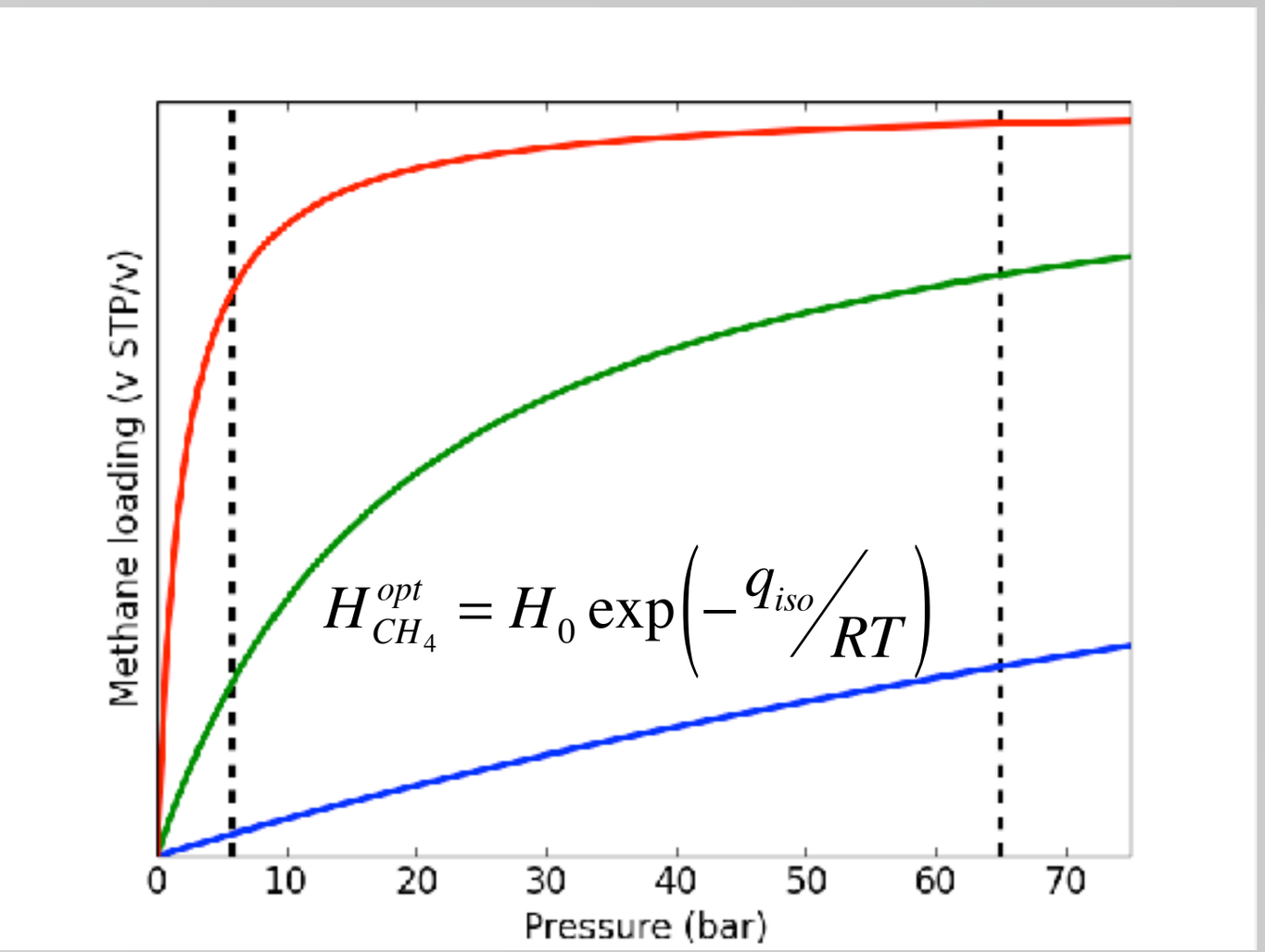

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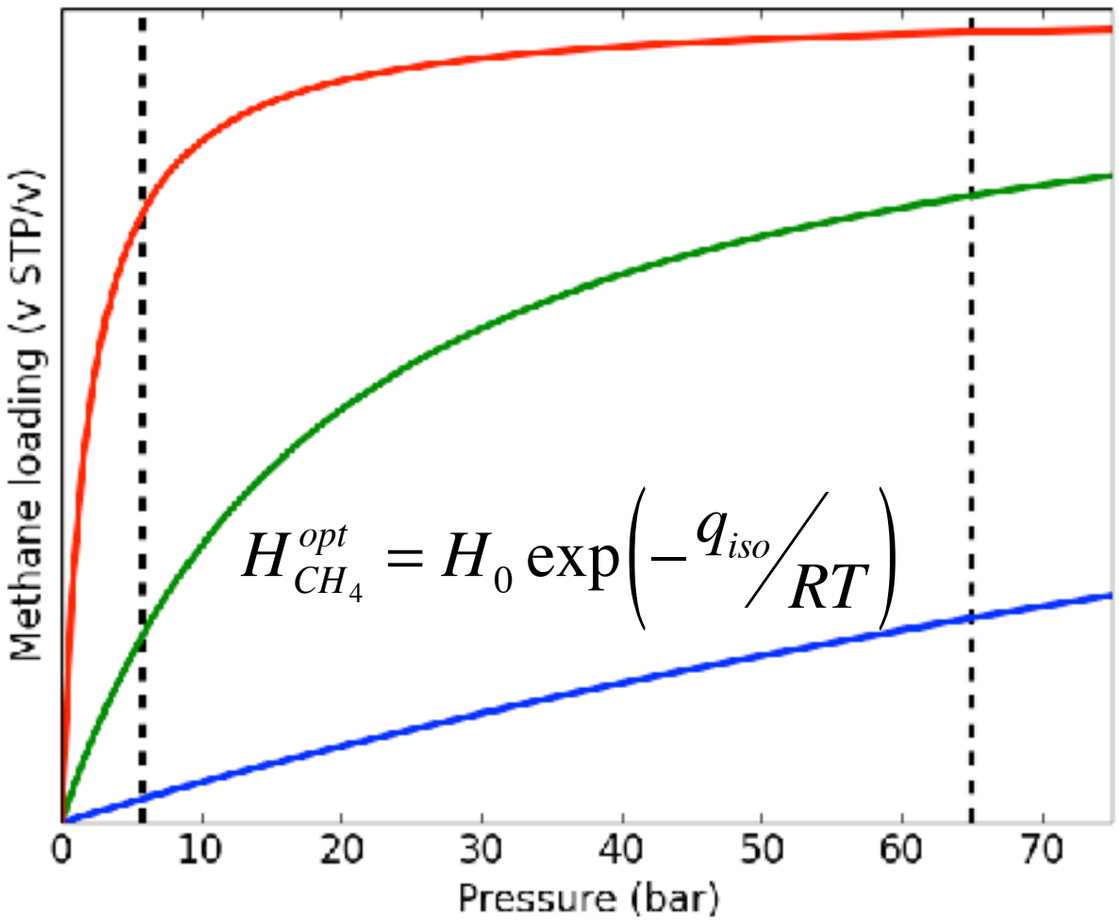

Langmuir 2006, *22*, 1688−1700

Optimum Conditions for Adsorptive Storage

Suresh K. Bhatia†

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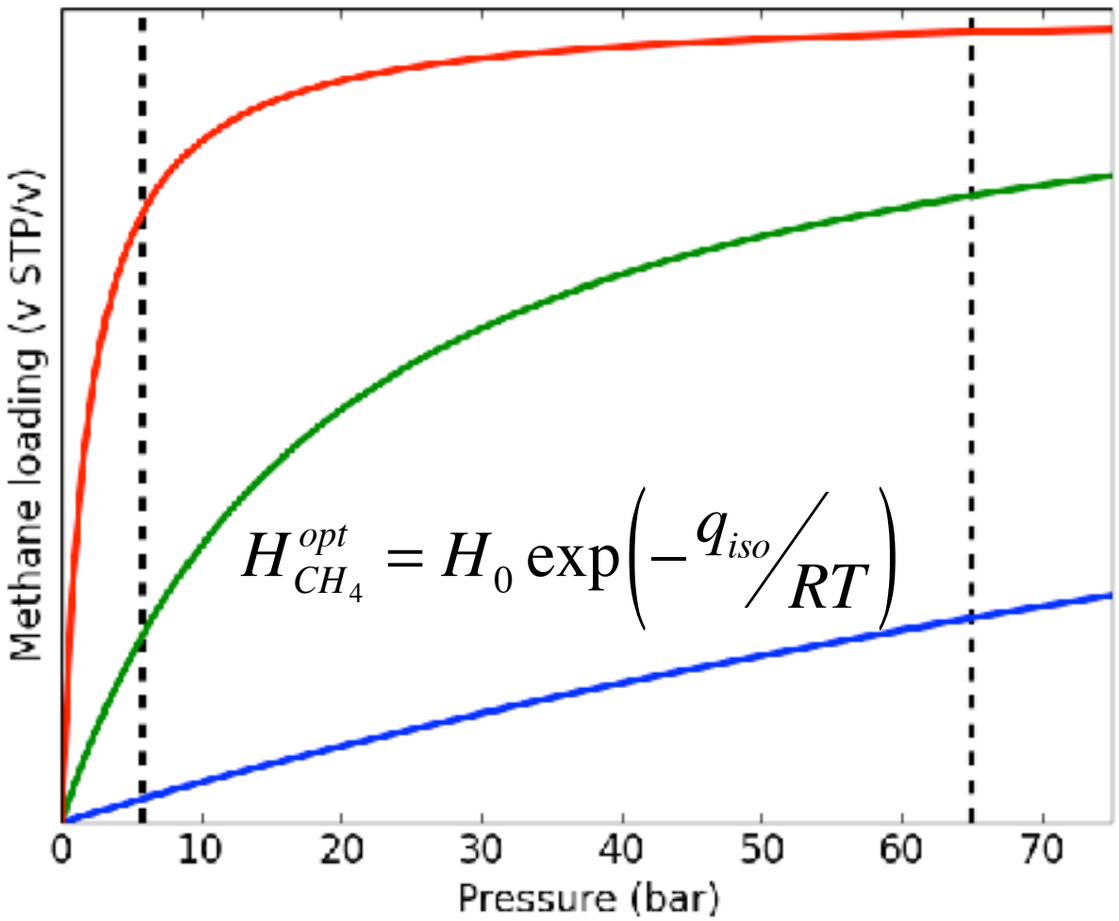
Alan L. Myers*

Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104

Goal: maximize deliverable capacity



"For methane, an optimal enthalpy change of [16.2] kJ/mol is found."

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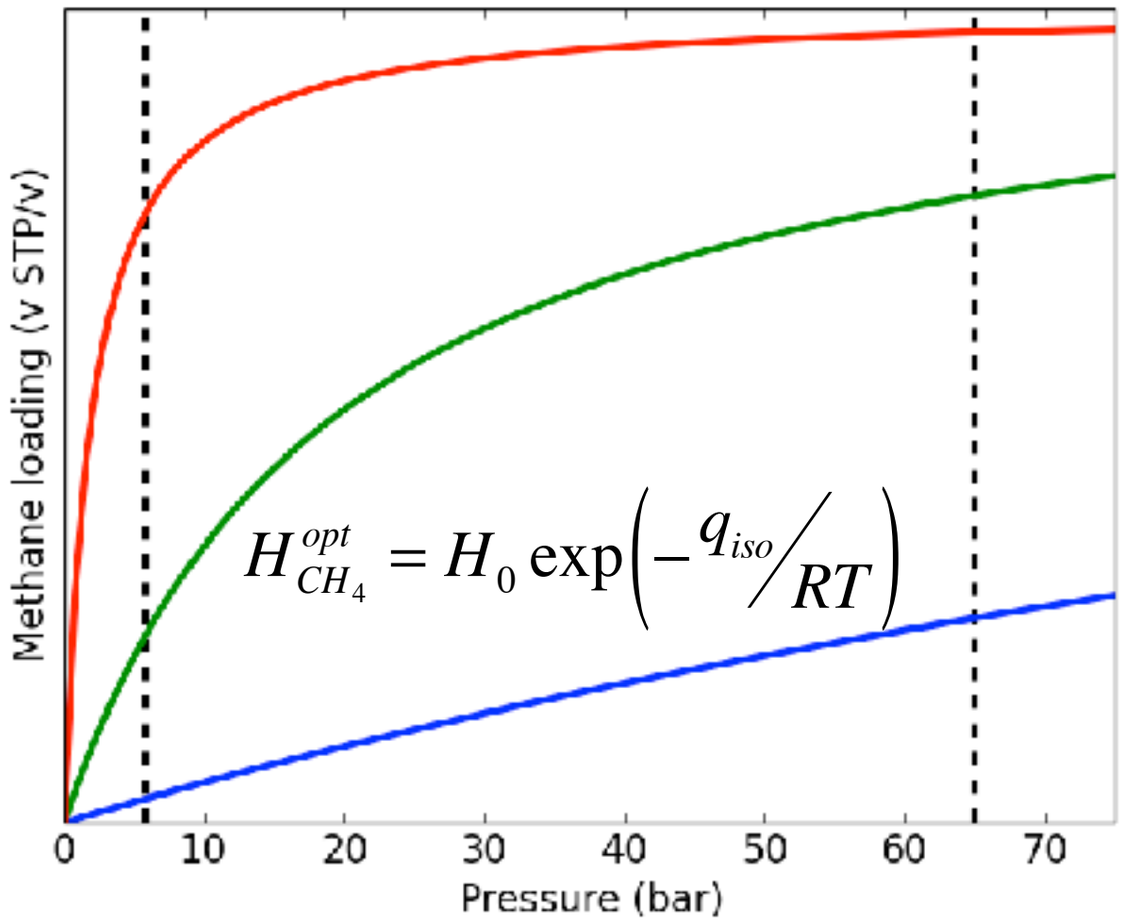

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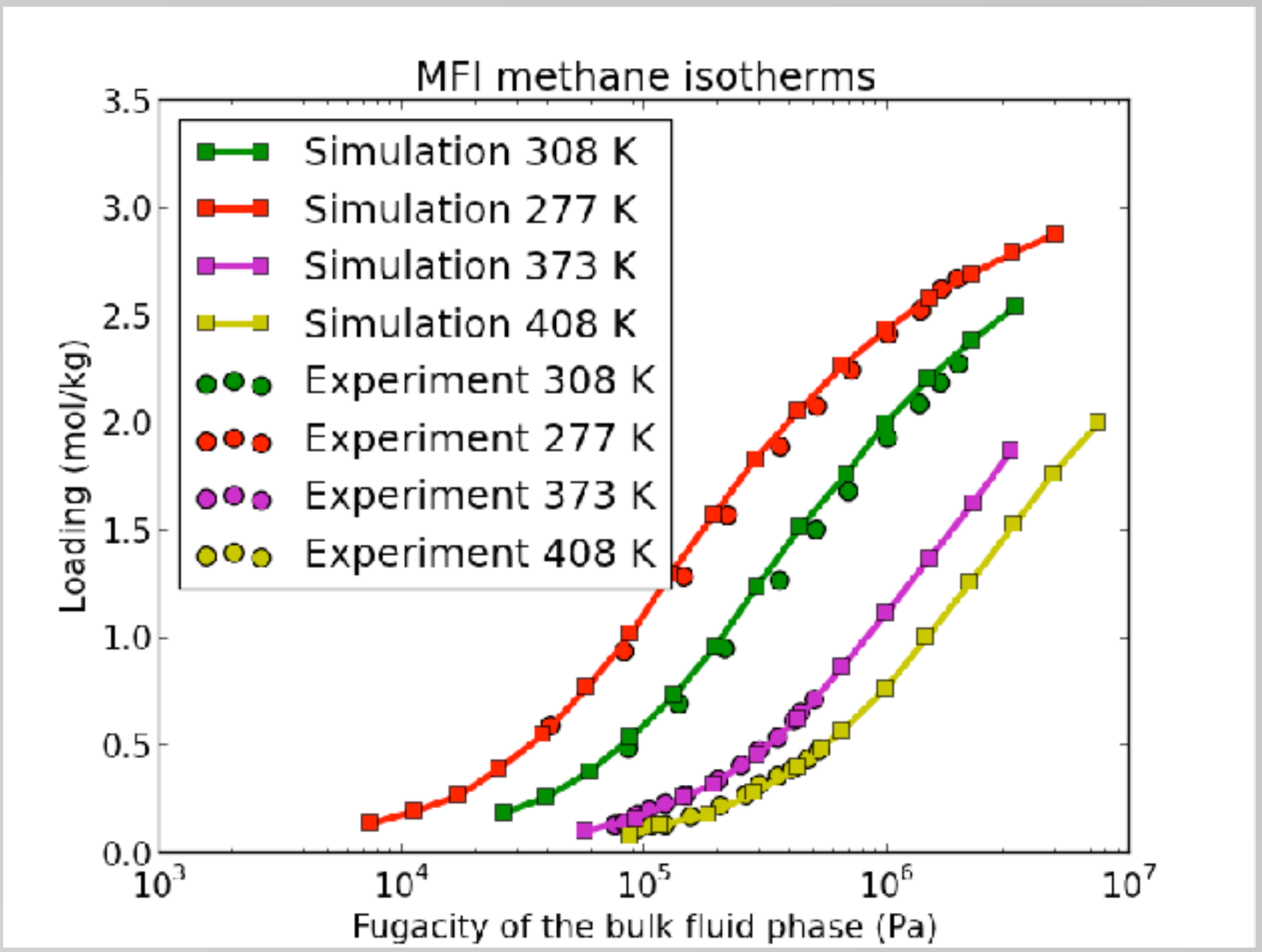
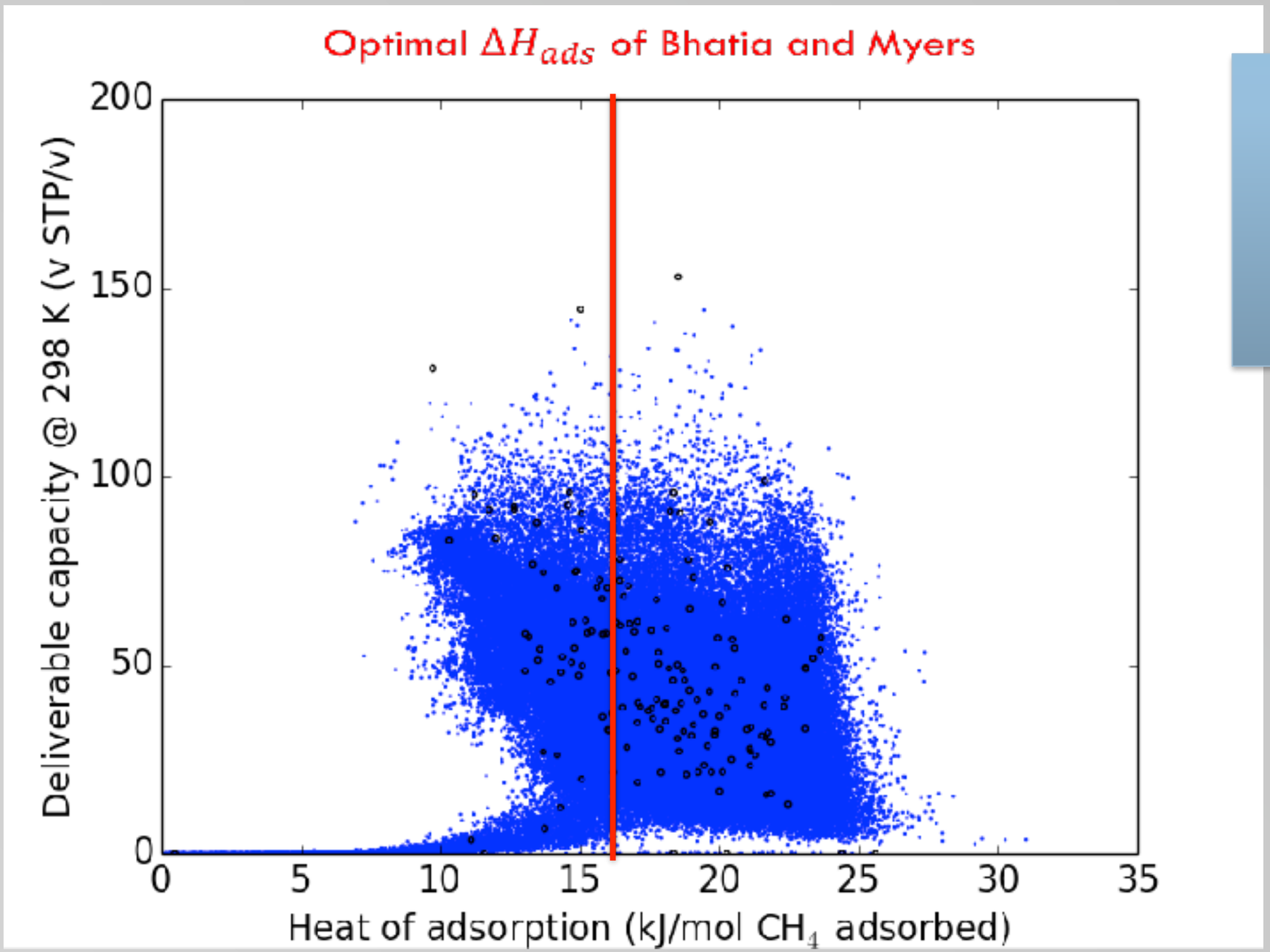
… but only a limited number of materials were analyzed

In silico screening of zeolites



MFI expt'l data: Sun *et al*. (1998) *J. Phys. Chem. B.* 102(8), 1466-1473.
Zhu *et al.* (2000) *Phys. Chem. Chem. Phys.* 2(9), 1989-1995.
Force field: Dubbeldam *et al*. (2004) *Phys. Rev.* 93(8), 088302.

In silico screening of zeolites



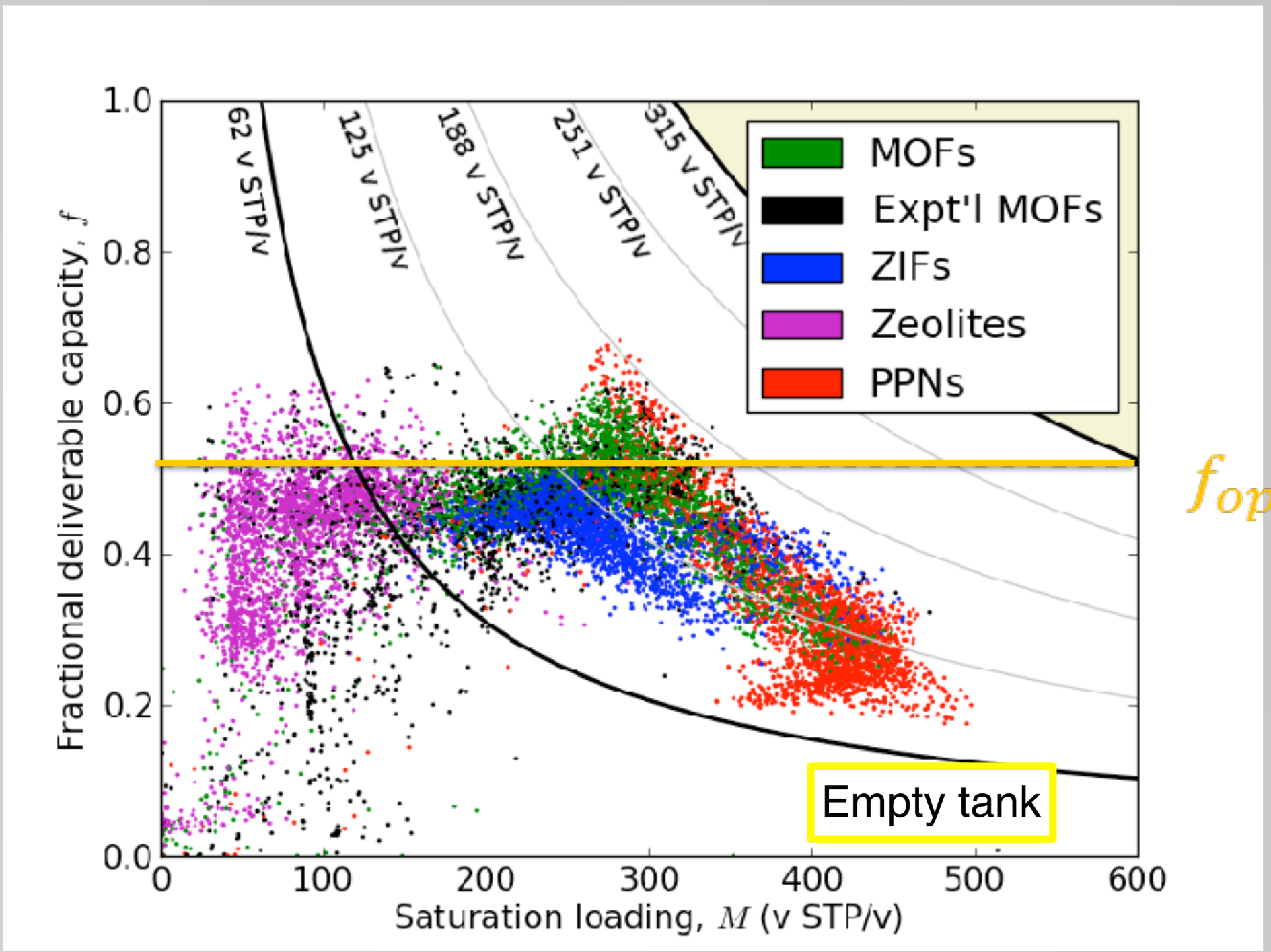
C. Simon *et al*. (2014) *Phys. Chem. Chem. Phys*. 16 (12), 5499-5513

Can we find a material that meets the DOE target?

Screening > 100,000 materials

- zeolites
- Metal organic Frameworks, MOFs (Snurr and co-workers)
- zeolitic imidazolate frameworks, ZIFs, (Haranczyk)
- Polymer Porous Networks, PPNs (Haranczyk)

Insight from the model



C. Simon, et al Energy Environ. Sci. **8**, 1190 (2015) http://dx.doi.org/10.1039/C4EE03515A

A theory of nothing

Methane storage in all silica zeolites:

- only the pore shape matters
- similar pores should have similar performance

Methane storage in all silica zeolites:

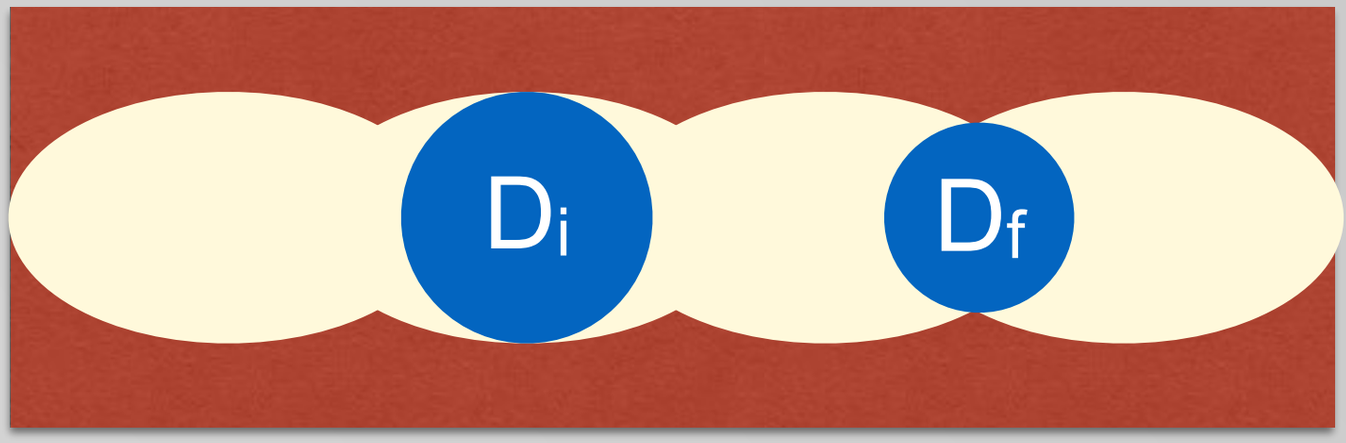
- only the pore shape matters
- similar pores should have similar performance

How to compare pores?

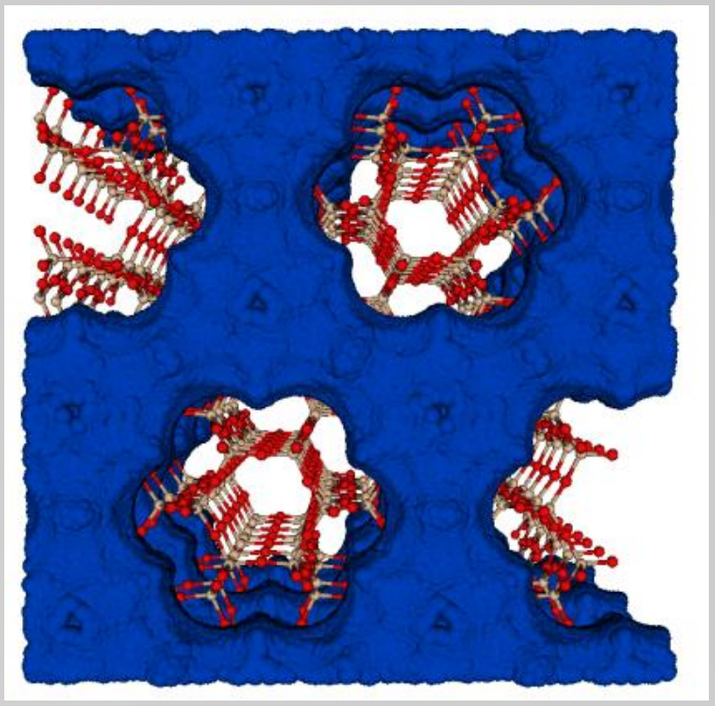
Simple Descriptors

Simple descriptors:

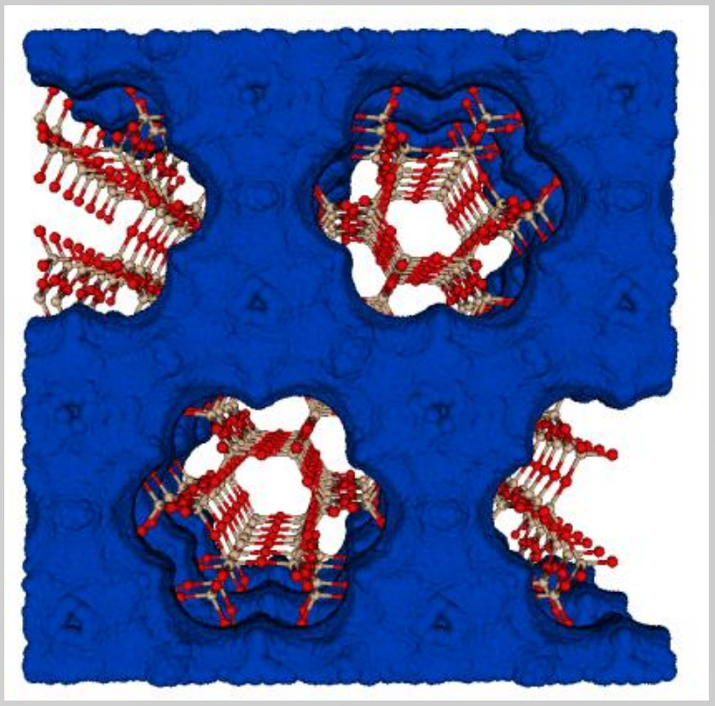
- D_i : diameter of maximum included sphere,
- D_f: diameter of maximum free sphere,
- ρ: density,
- ASA: accessible surface area,
- AV: accessible volume



SSF

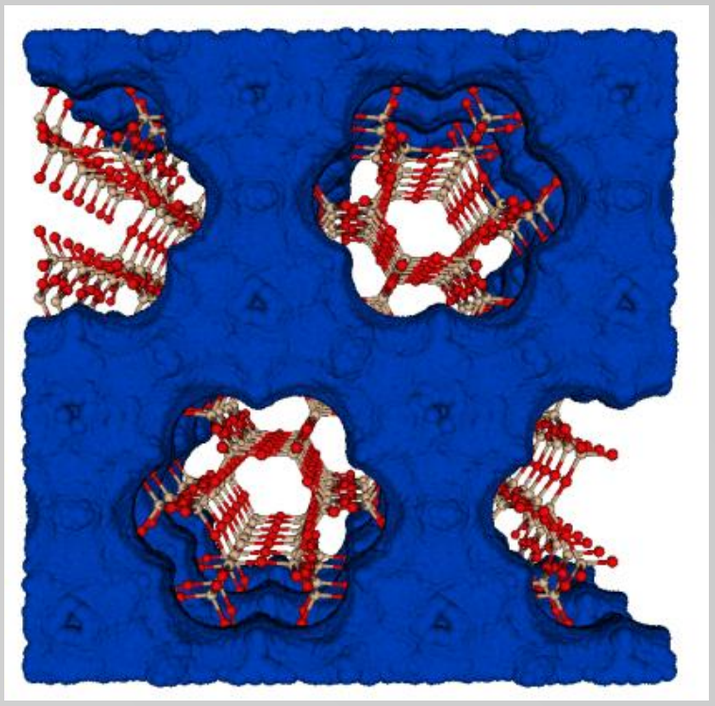


SSF

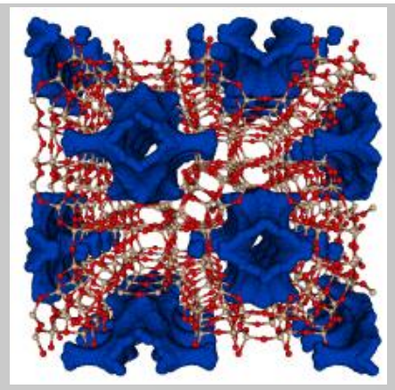


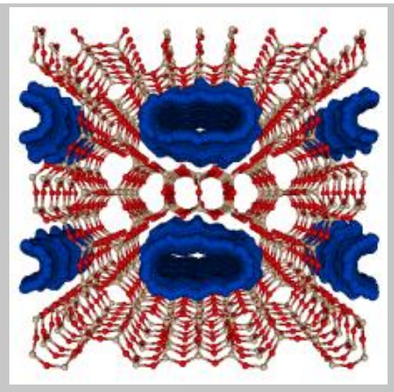
		name	D_i	D_f	ρ	ASA	AV
CD	Seed	SSF	7.59	6.15	1.64	1191	0.122
	1st	h8242590	7.87	6.16	1.62	1210	0.119
	2nd	h8239380	7.60	6.29	1.63	1156	0.120
	3rd	h8267258	7.72	6.21	1.63	1205	0.115
	4th	h8070132	7.69	6.49	1.62	1187	0.126

SSF



ConD





		name	D_i	D_f	ρ	ASA	AV
CD	Seed	SSF	7.59	6.15	1.64	1191	0.122
	1st	h8242590	7.87	6.16	1.62	1210	0.119
	2nd	h8239380	7.60	6.29	1.63	1156	0.120
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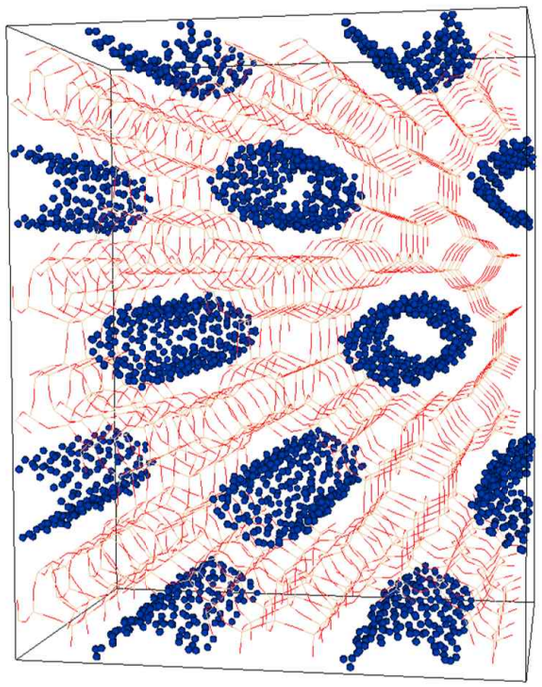
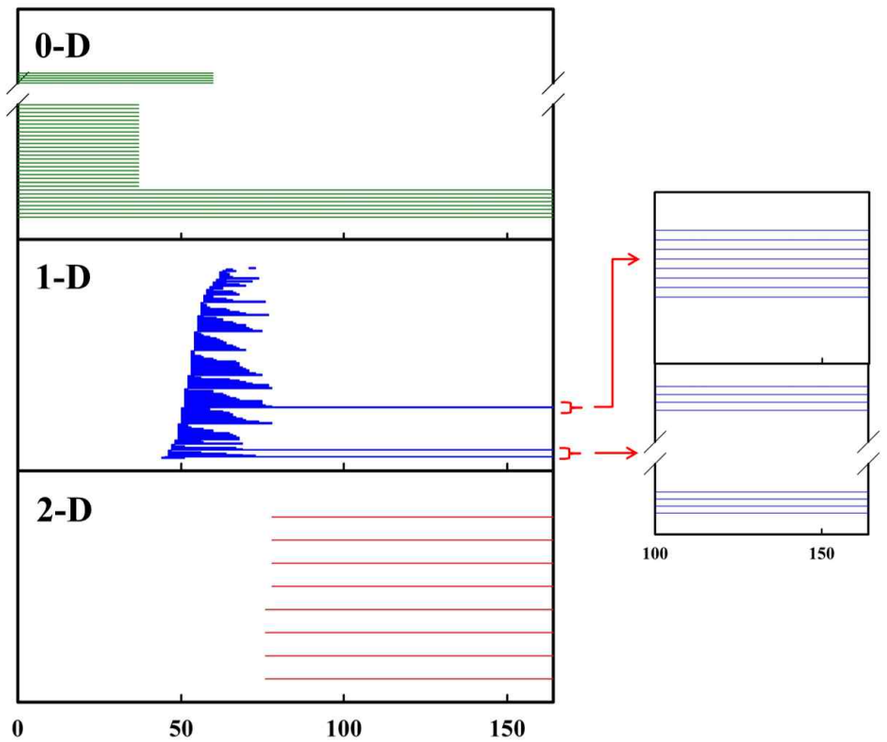
	4th	h8070132	7.69	6.49	1.62	1187	0.126

Persistent Homology

DON





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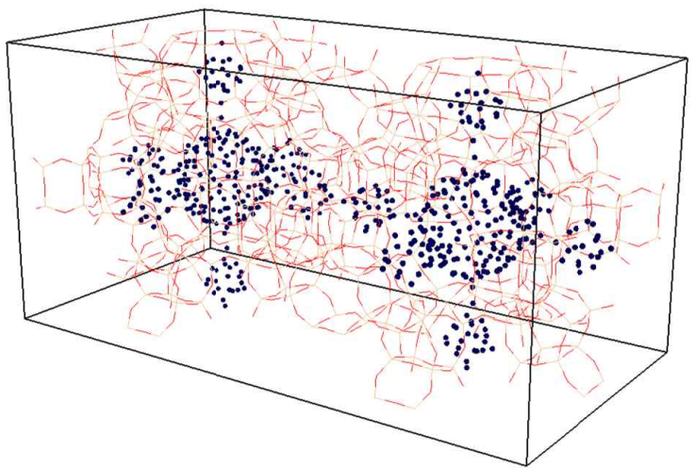

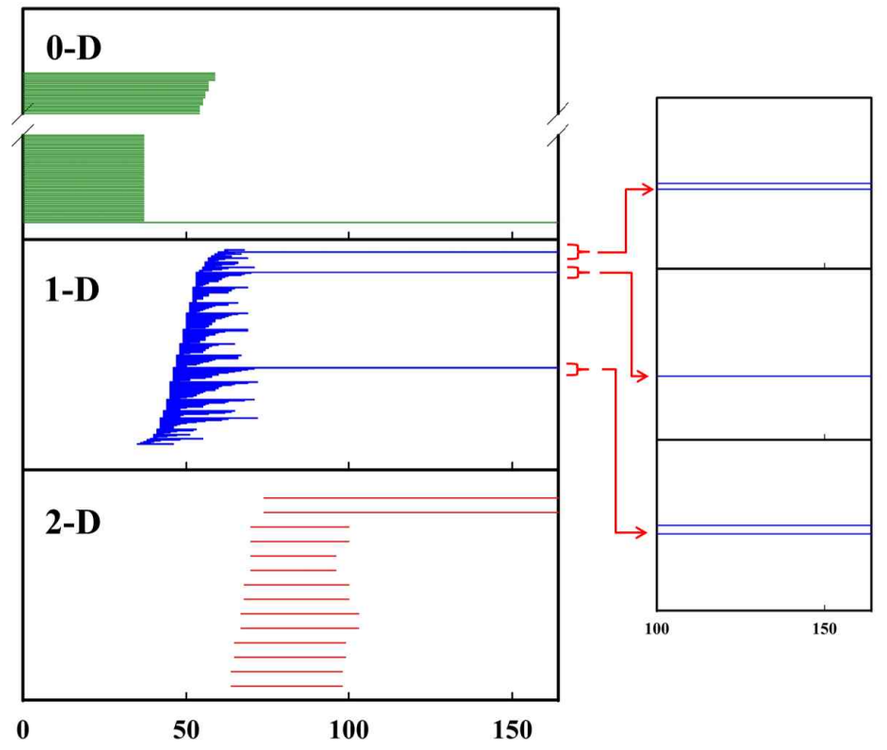

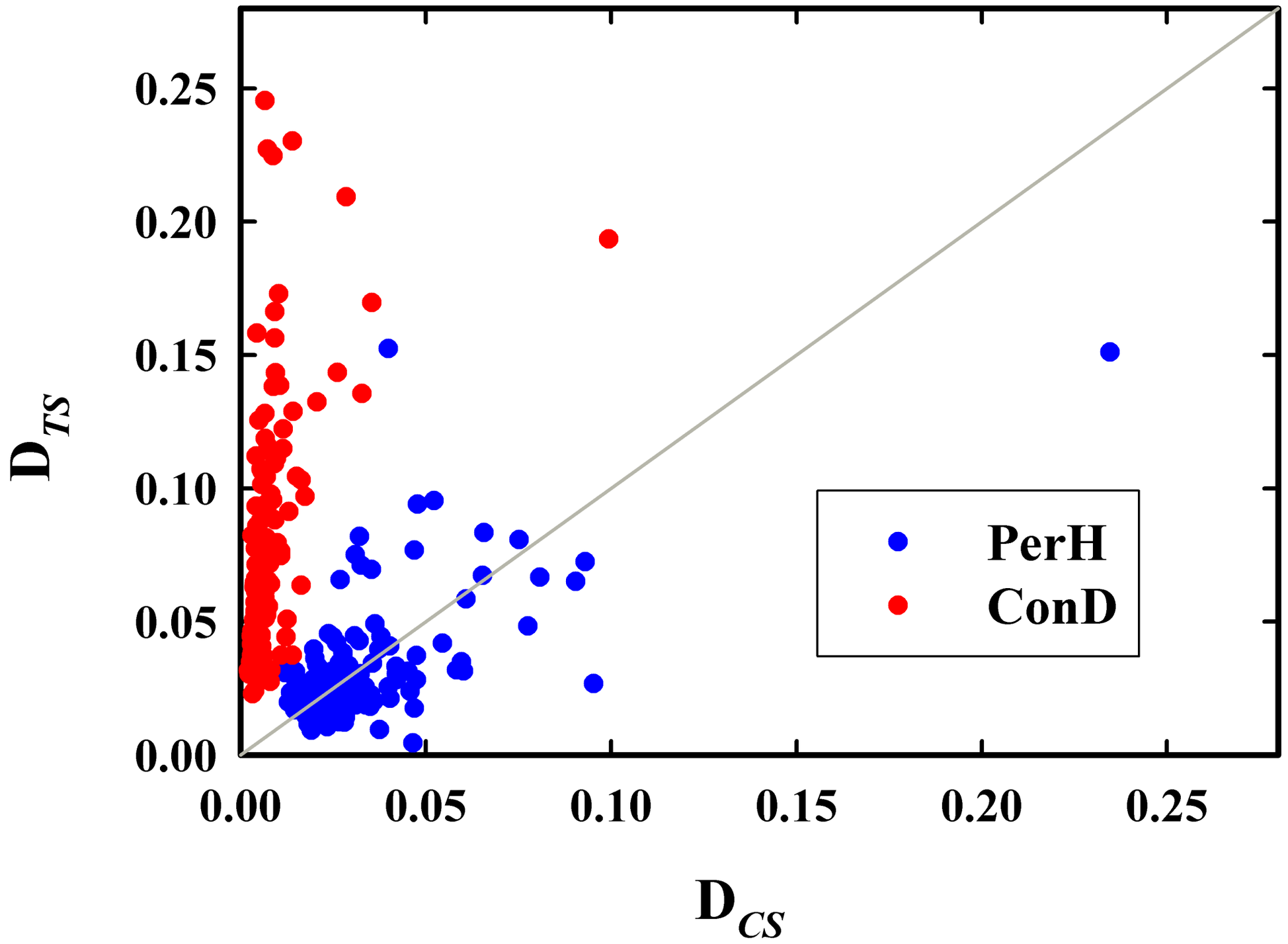
0.25
0.20
0.15
0.10
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0.00
0.00
0.05
0.10
0.15
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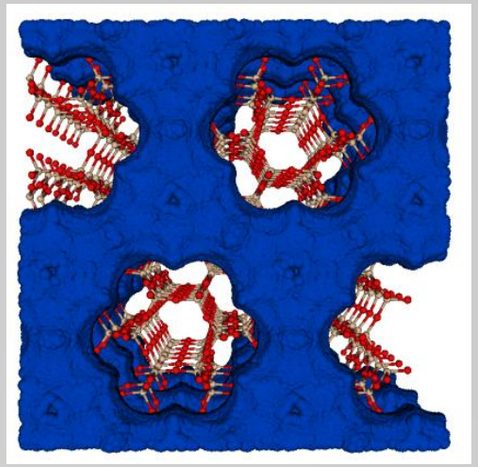
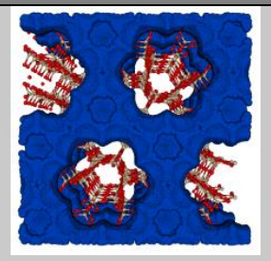
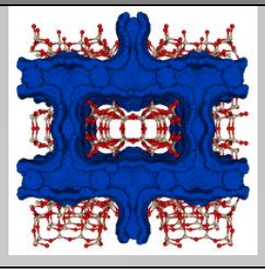
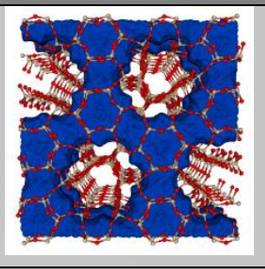
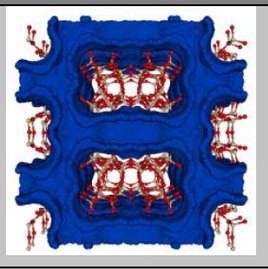
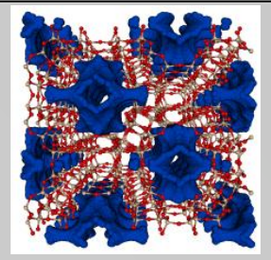
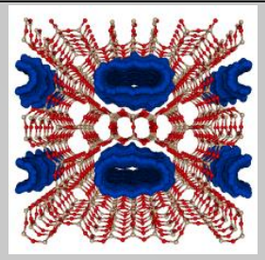
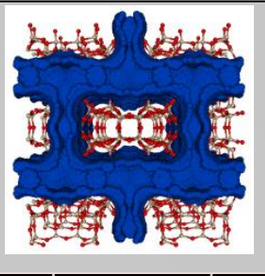
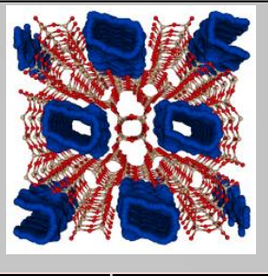
0.25
D_TS
D_CS
PerH
ConD

		name	D_i	D_f	ρ	ASA	AV
TD	Seed	SSF	7.59	6.15	1.64	1191.97	0.122
	1st	h8328603	8.09	6.34	1.77	1167.86	0.120
	2nd	h8267258	7.72	6.21	1.63	1205.27	0.115
	3rd	h8325096	7.28	5.91	1.72	1160.44	0.114
	4th	h8267032	7.54	6.22	1.70	1171.01	0.115
CD	Seed	SSF	7.59	6.15	1.64	1191.97	0.122
	1st	h8242590	7.87	6.16	1.62	1210.05	0.119
	2nd	h8239380	7.60	6.29	1.63	1156.76	0.120
	3rd	h8267258	7.72	6.21	1.63	1205.27	0.115

Seed	Descriptor	Selected Nth Similar Structure			
		1st	2nd	3rd	4th
SSF 	PerH				
	ConD				

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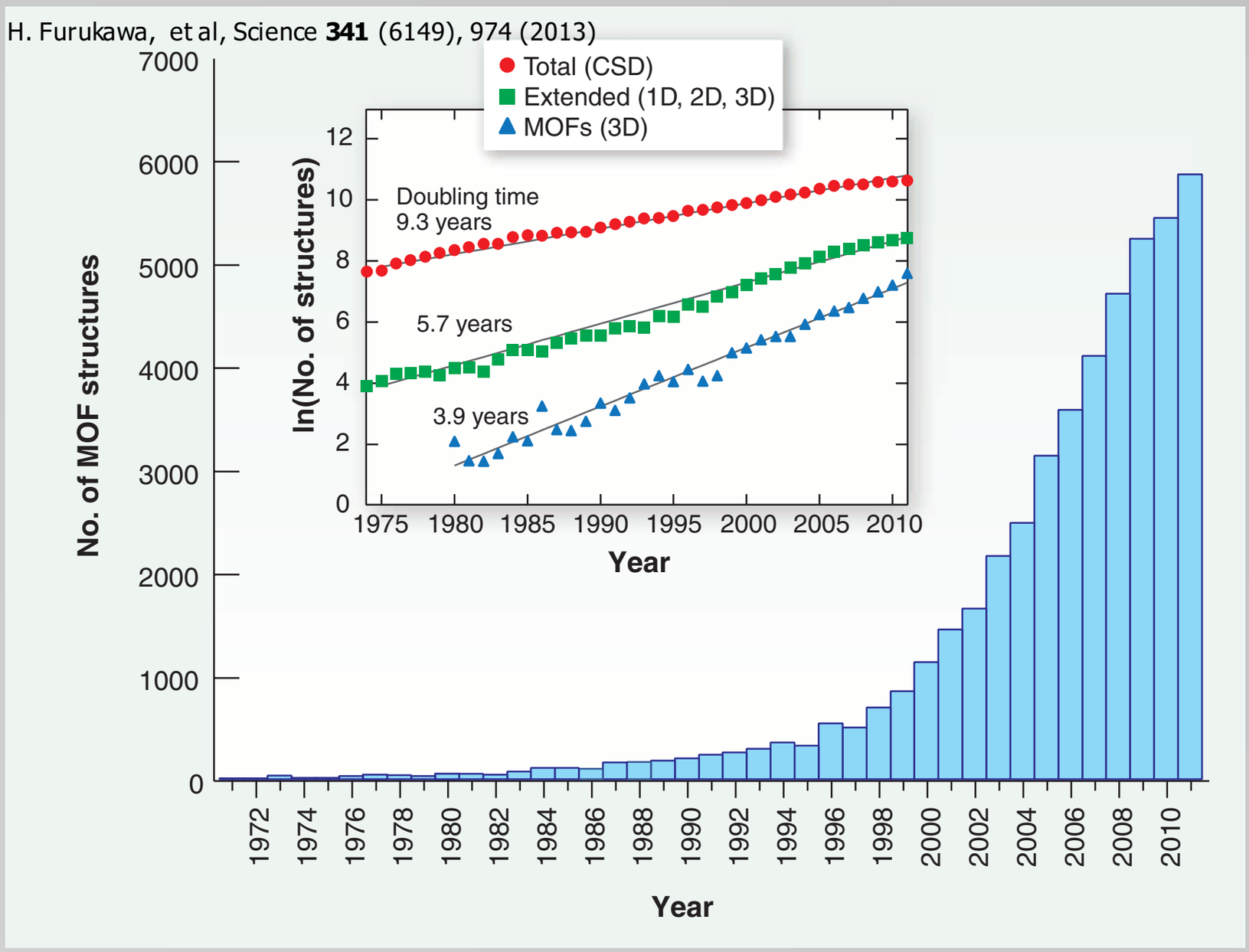
	2nd	h8239380	7.60	6.29	1.63	1156.76	0.120
	3rd	h8267258	7.72	6.21	1.63	1205.27	0.115

Big data: too many materials

Question: has a MOF with a similar pore structure already been published?

Current technique:
compare by eye



Criteria:

- MOFs published and structures deposited in the CSD
- Structures are very similar
- MOFs do not have the same name
- Published in different articles
- Different authors
- No cross-references

27 hits of too similarity

Y. Lee, et al. Nat. Commun. **8** (2017) http://dx.doi.org/10.1038/ncomms15396

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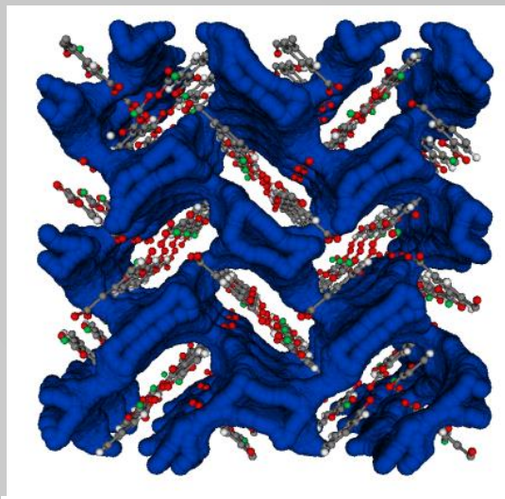
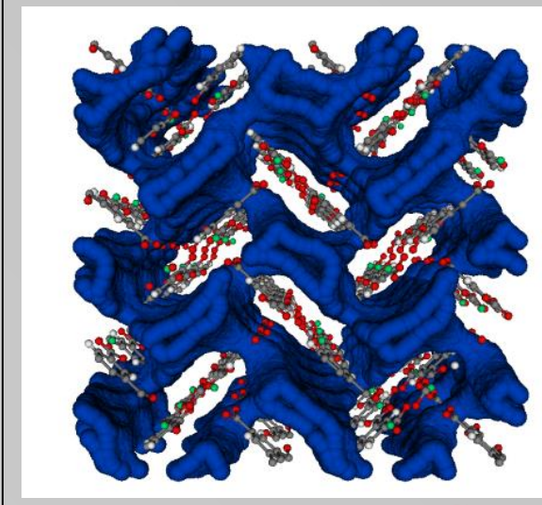
AFUPEX



Gaodeng Xuexiao Huaxue Xuebao, 2007, 28, 1437

SEHSUU



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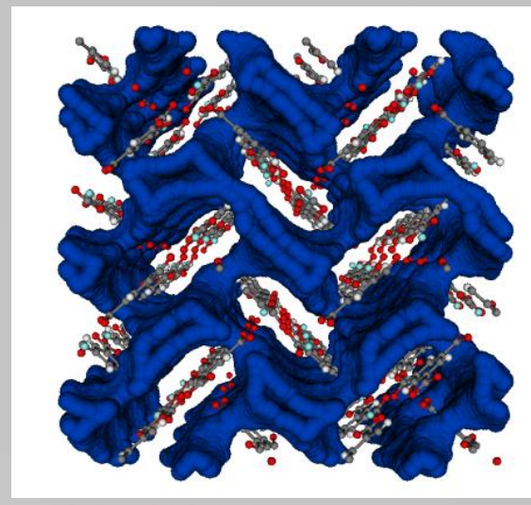

Inorg. Chem. 45, 4065 (2006)

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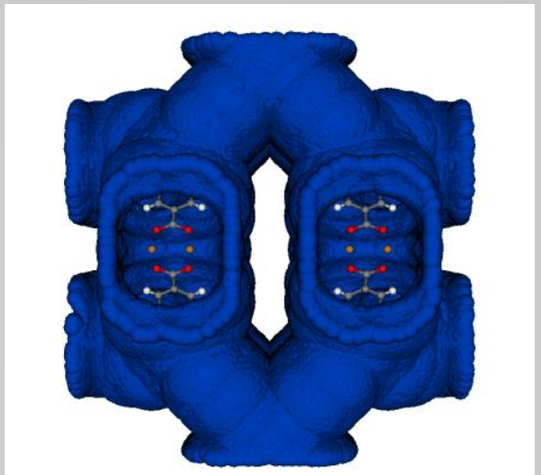

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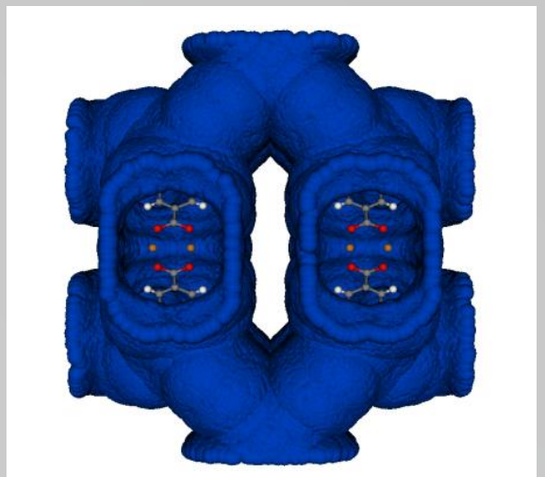

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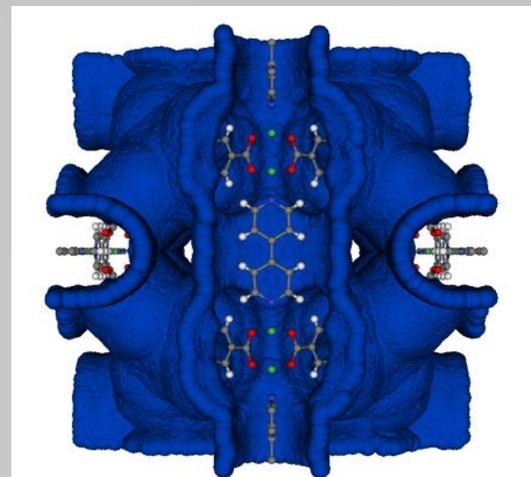
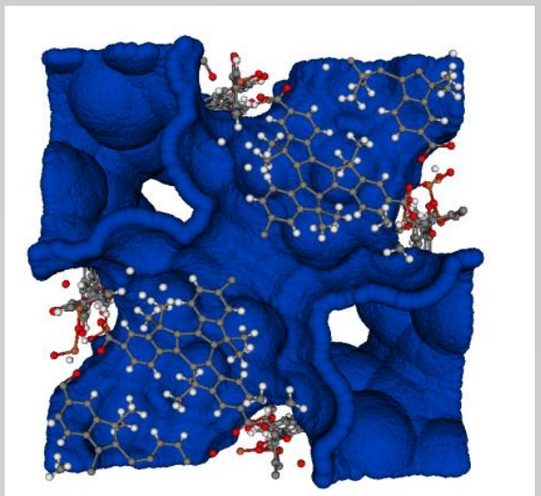


Chem. Eur. J. 17, 13007 (2011)

VETTIZ



Chem. Eur. J. 18, 16642 (2012)

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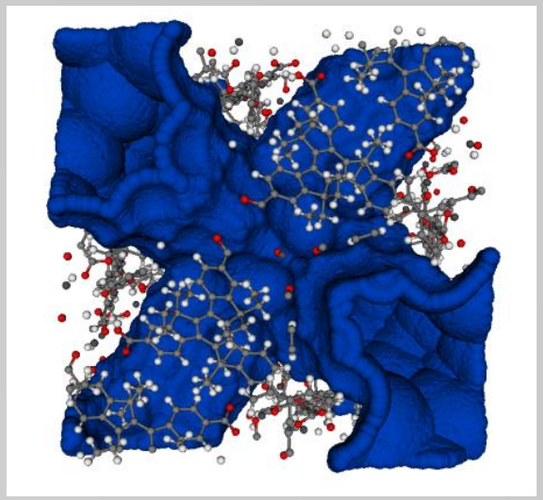

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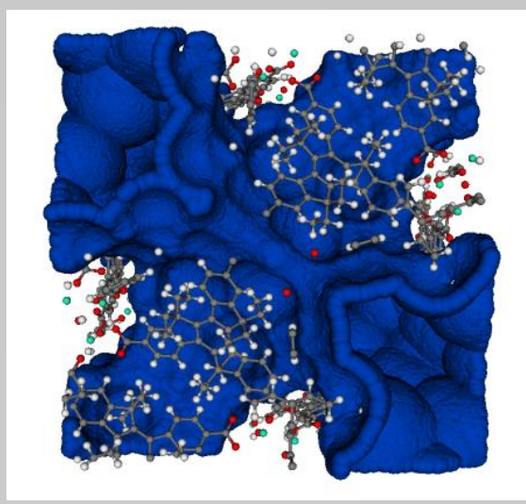
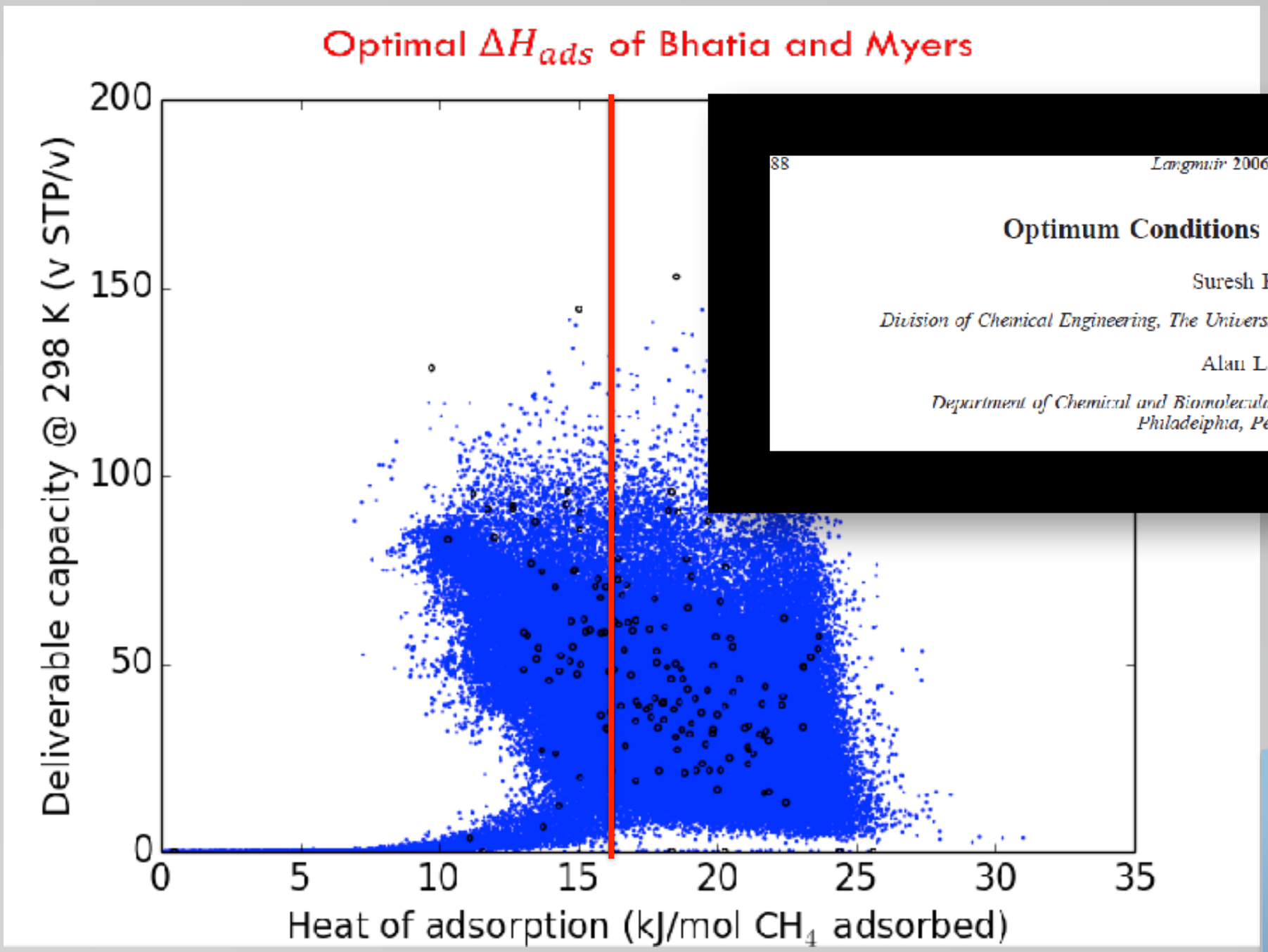


J. Am. Chem. Soc. 131, 3814 (2009)

Methane Storage
(part 2)

In silico screening of zeolites



88 *Langmuir* 2006, *22*, 1688−1700

Optimum Conditions for Adsorptive Storage

Suresh K. Bhatia†

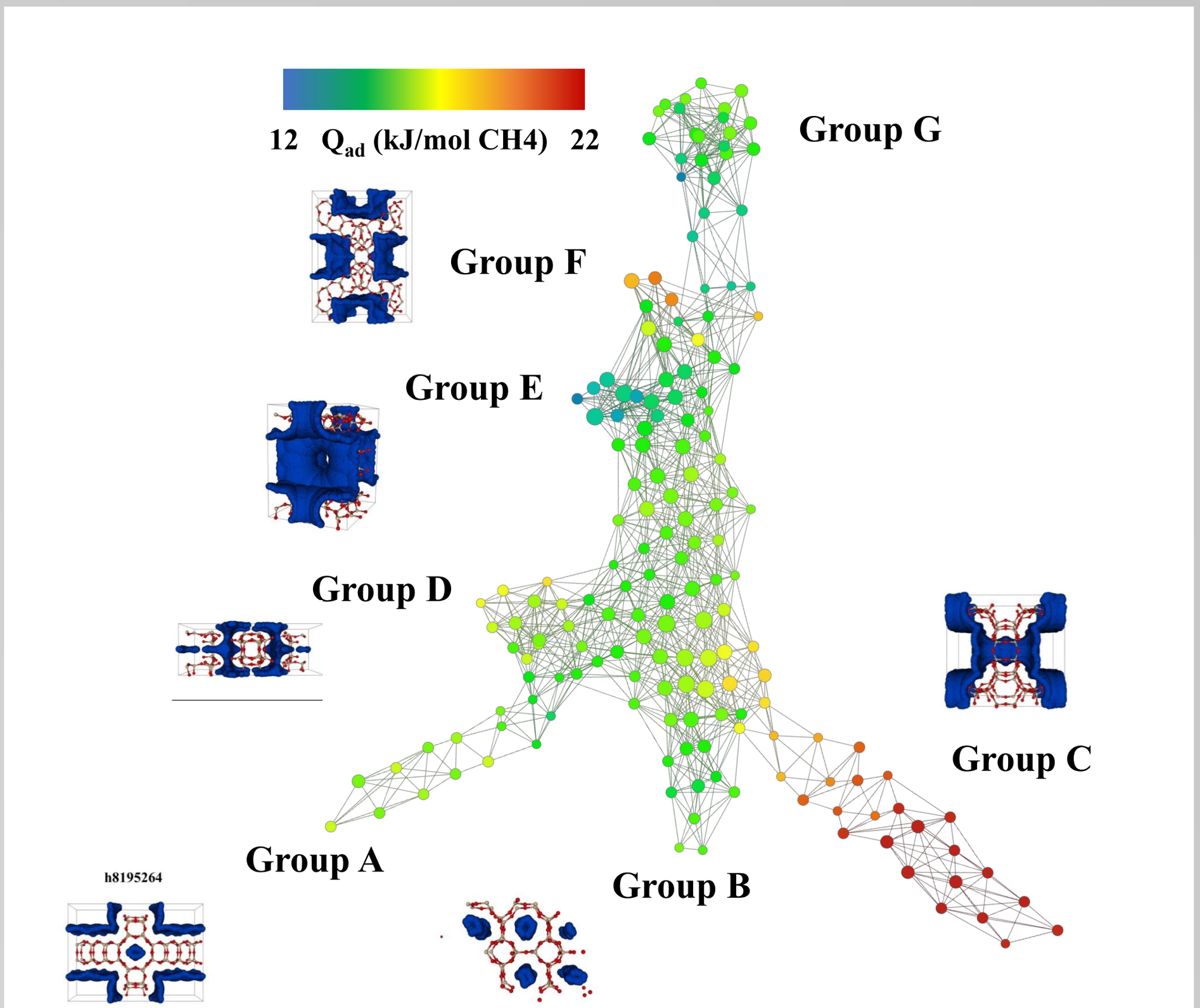
Division of Chemical Engineering, The University of Queensland, Brisbane, QLD 4072

Alan L. Myers*

Department of Chemical and Biomolecular Engineering, University of Pennsylvania Philadelphia, Pennsylvania 19104

C. Simon *et al*. (2014) *Phys. Chem. Chem. Phys*. 16 (12), 5499-5513

Heat of a adsorption of top performing materials



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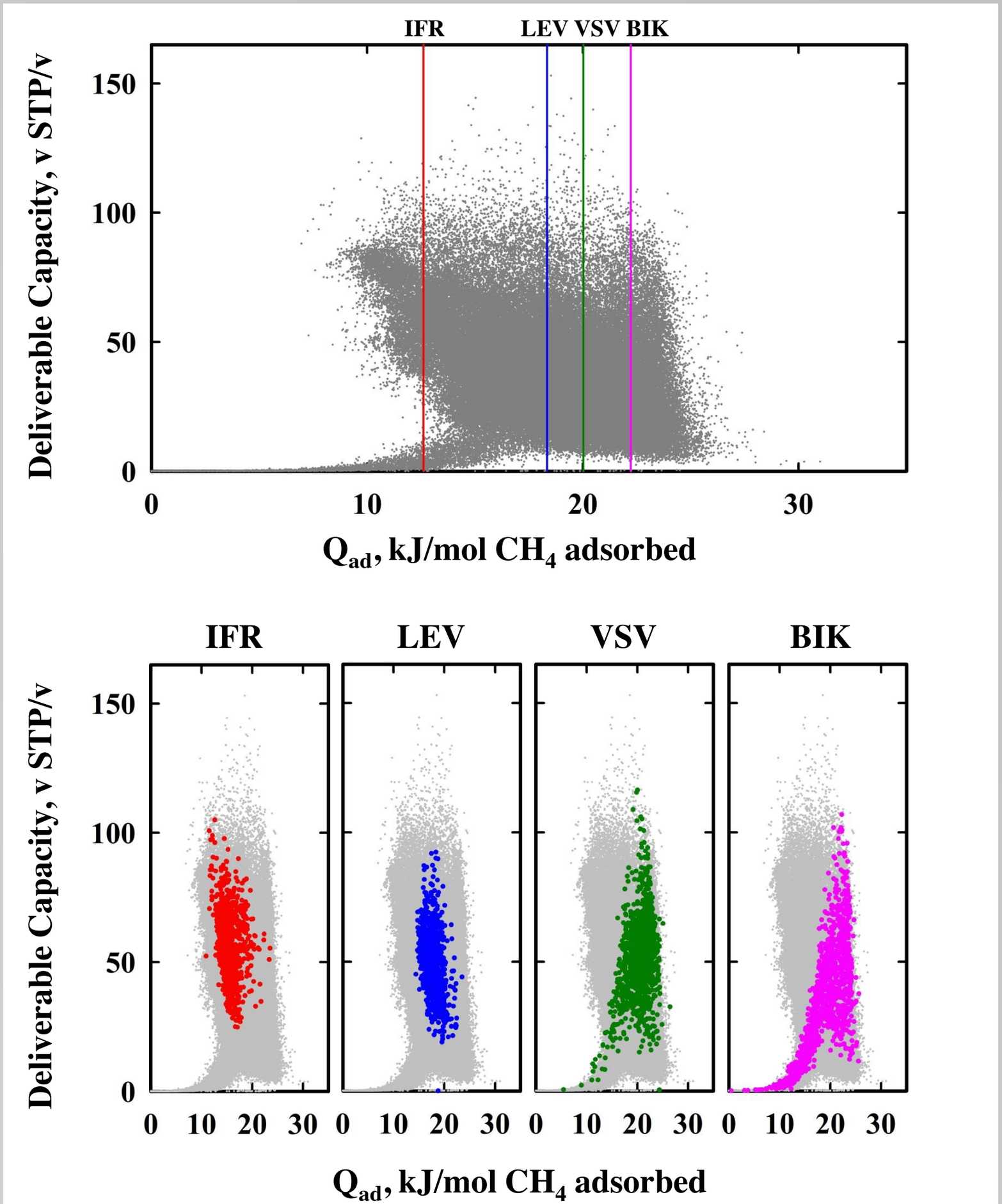
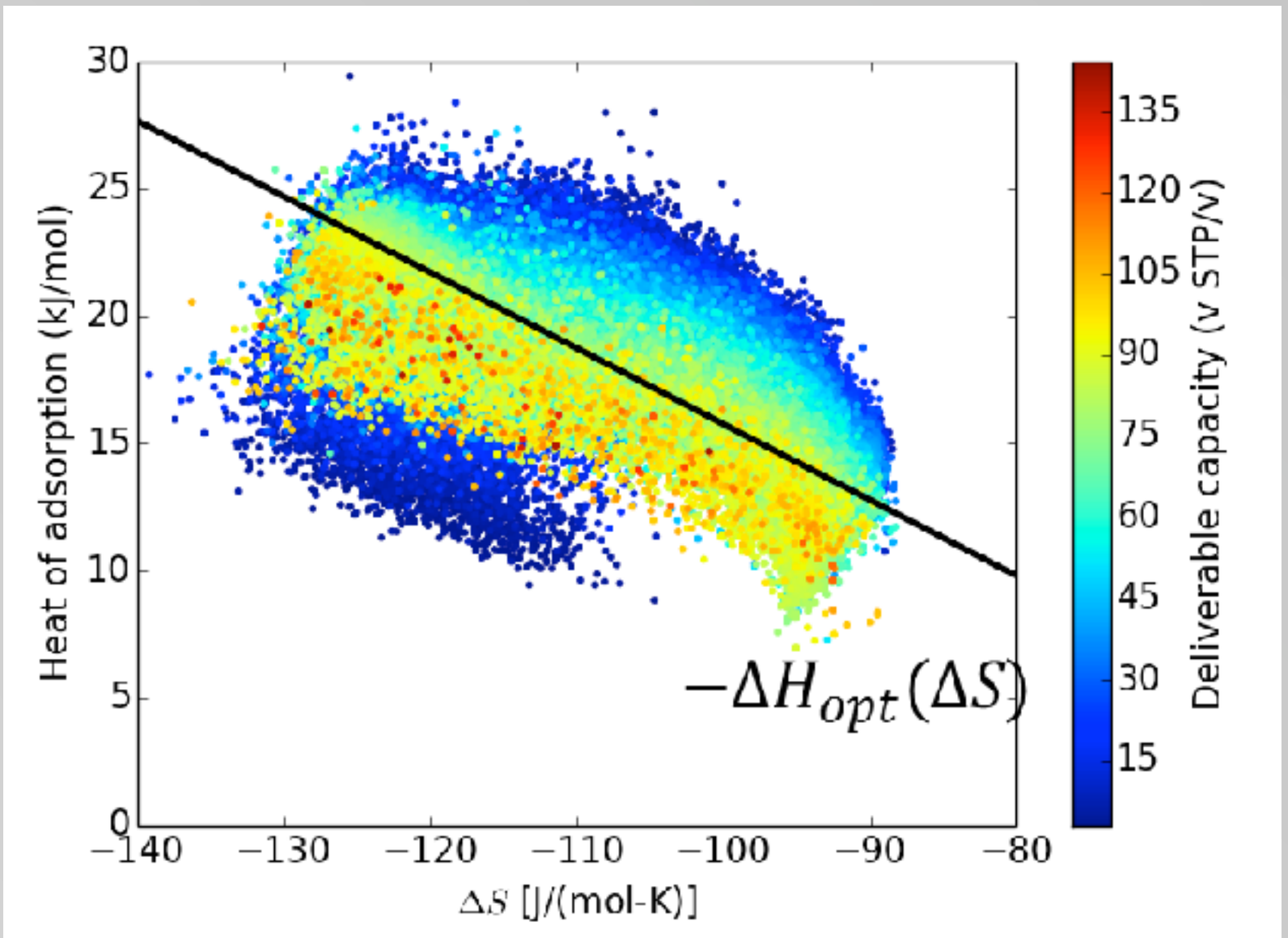


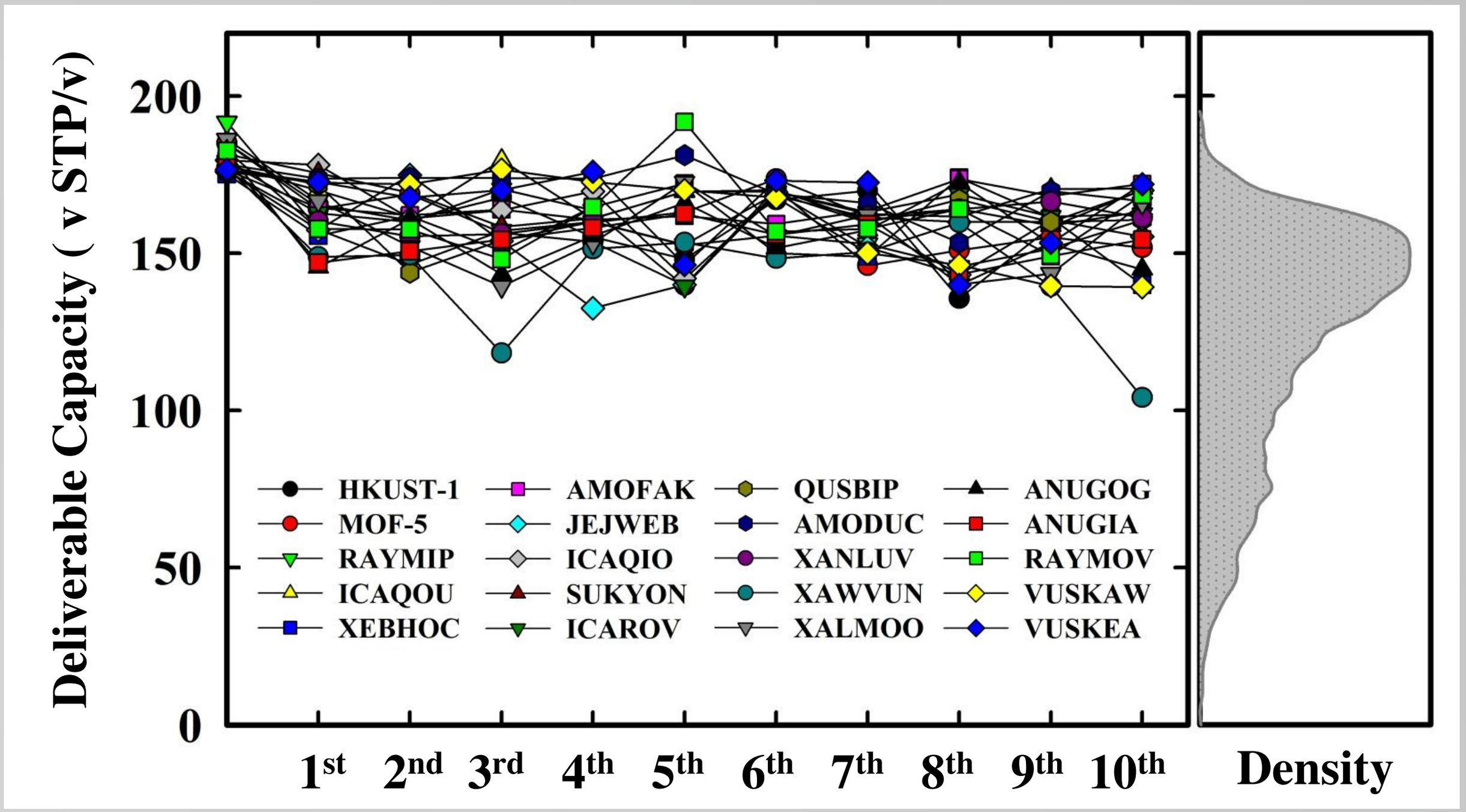
Y. Lee, et al. Nat. Commun. **8** (2017) http://dx.doi.org/10.1038/ncomms15396

Enthalpy vs. entropy

- ΔS not the same for all materials
- Wide range of ΔH that yields optimal material



Similar materials have similar performance



Y. Lee, et al. Nat. Commun. **8** (2017) http://dx.doi.org/10.1038/ncomms15396

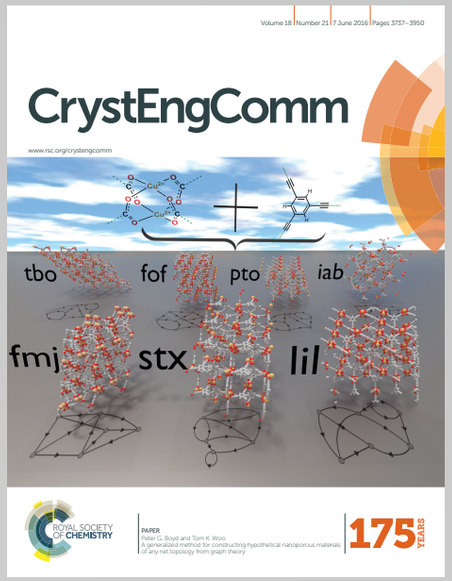
The diversity of nothing

A simple question

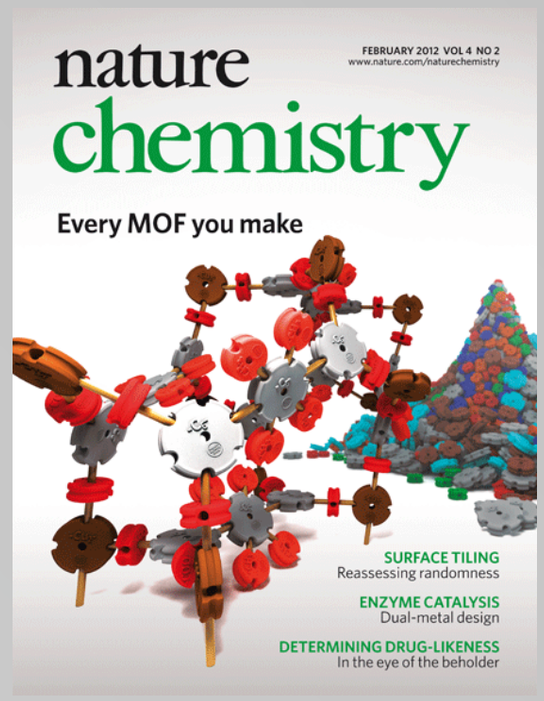
Databases:

- Experiments
- Randy Snurr and co-workers
- Pete Boyd and co-workers

Chung, Y. G. *et al.*. *Chem Mater* **26**, 6185-6192, (2014)



P. G. Boyd and T. K. Woo, Cryst Eng Comm **18** (21), 3777 (2016)



C. E. Wilmer, M. Leaf, C. Y. Lee, O. K. Farha, B. G. Hauser, J. T. Hupp, R. Q. Snurr, *Nat Chem* **2012**, *4*, 83-89.

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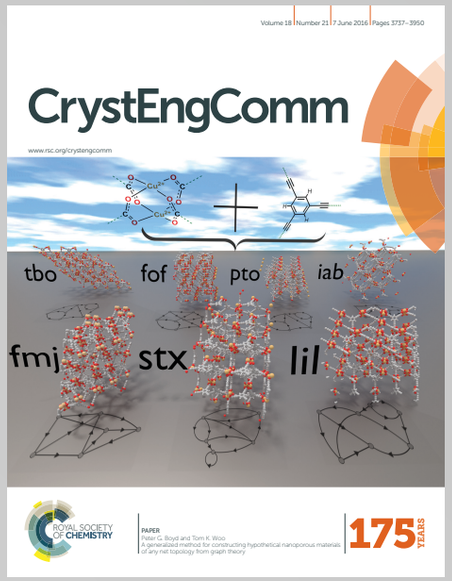

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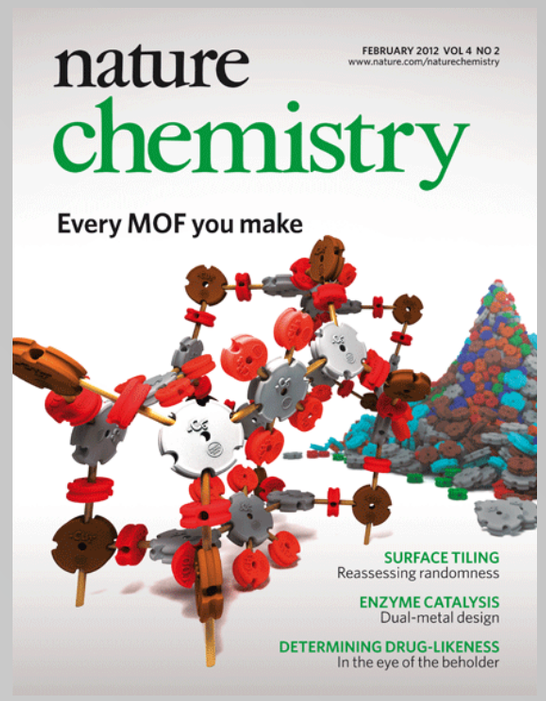

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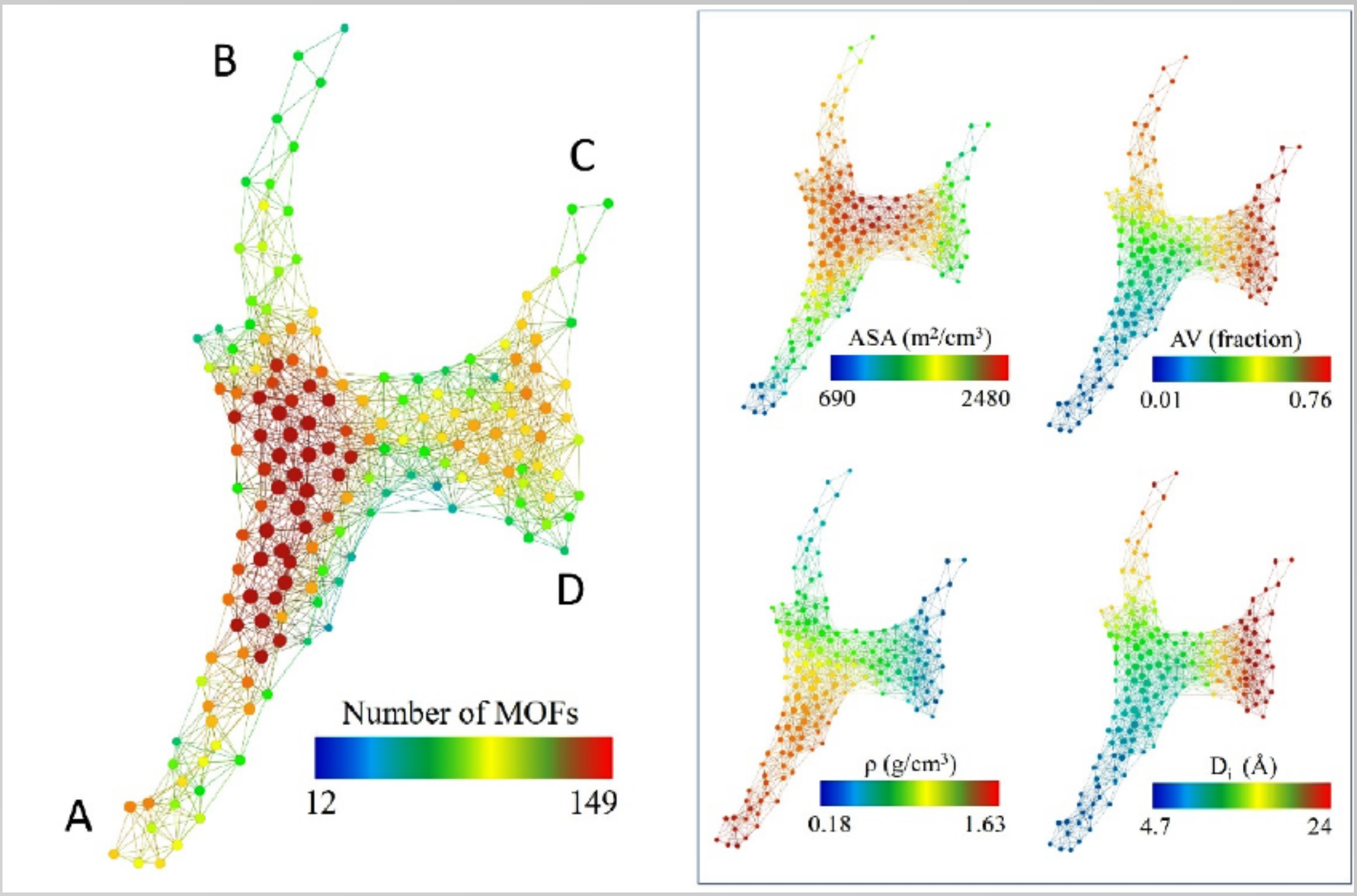
Who has the best nanoporous materials database?

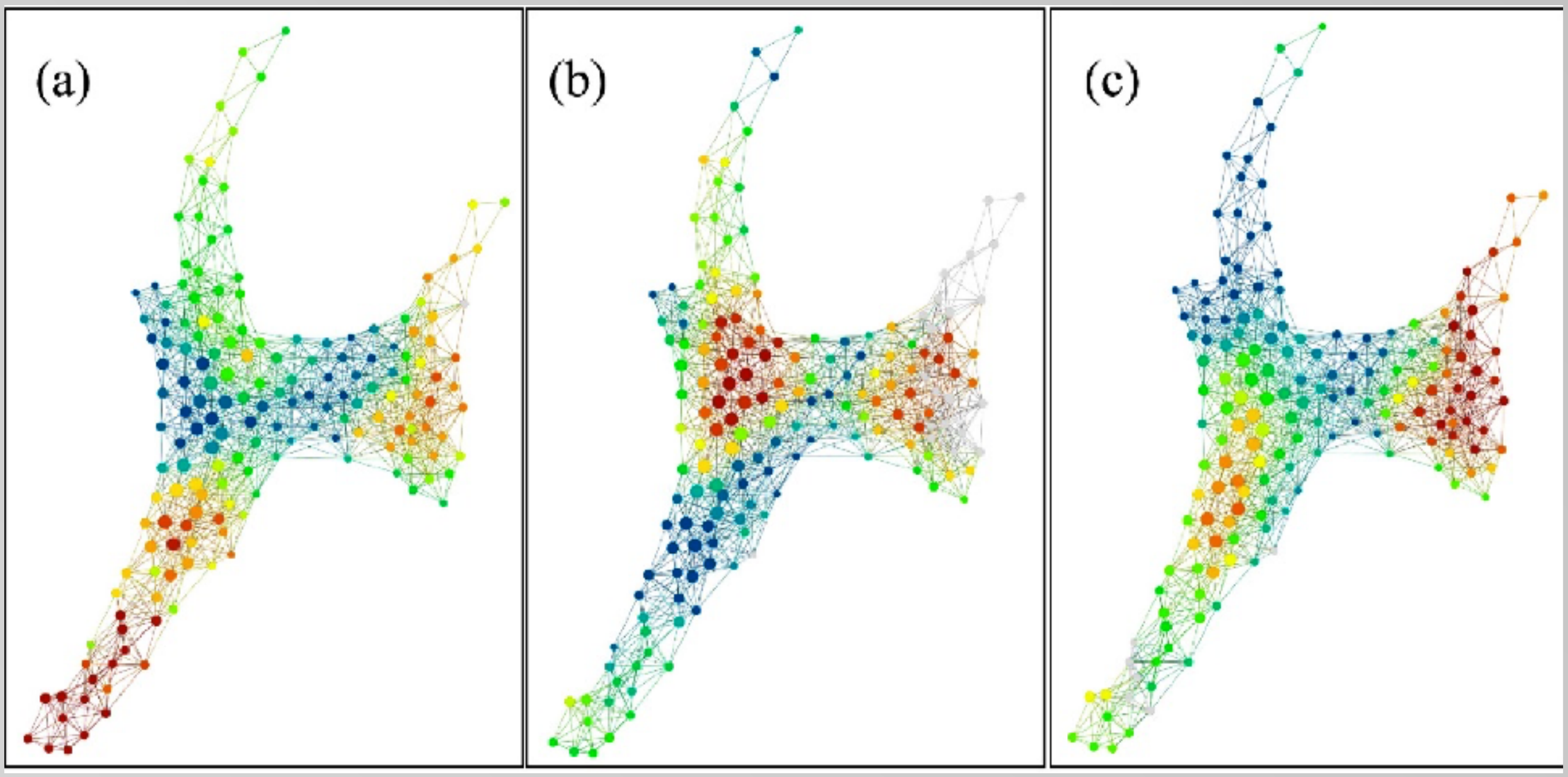
Diversity of MOF Materials Database



Five Different Types

Diversity of Materials Databases

Coverage of each DB on the entire map : red – high number, blue – low number, gray - empty



Experiments Snurr *et al.* Boyd *et al.*

Conclusions

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- **<u>Xe/Kr separations</u>**
  - sometimes you can be lucky …

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- **<u>Materials Genome</u>:**
  - Intelligence versus brute force ....
  - Screening for best materials: what can be obtained
  - Big-data science