The Materials Genome in Action

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Cluster trees, near neighbor graphs, and continuum percolation

A statistical approach to topological data analysis

Topological Graphs for Data Analysis: Structure, Stability and Statistics

Minimal geodesics along volume preserving maps, through semi-discrete optimal transport

The Materials Genome in Action

Triangulating manifolds

Zigzag persistence: New horizons in topological data analysis

Interactive visualization of high dimensional data: can we deal with curse of dimentionality and failure of intuition?

Suddenly, Professor Liebowitz realizes he has come to the seminar without his duck.

Acknowledgement

- **Materials Genome**
  - Cory Simon and Rocio Mercado (UC Berkeley
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  - Michael W. Deem (Rice)
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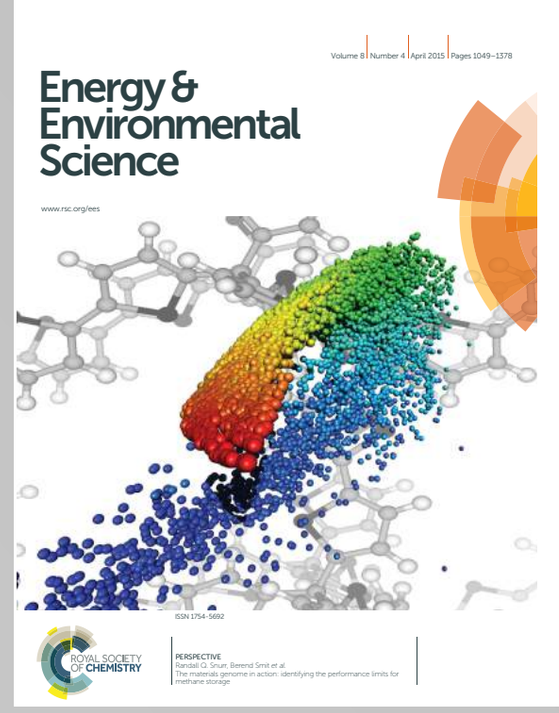
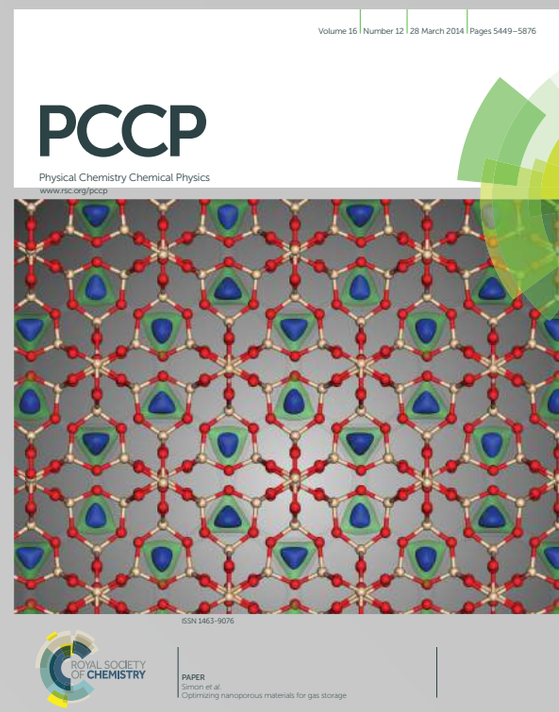
  - ERC-Adv, US Department of Energy, MARVEL (NCCR-SNF)

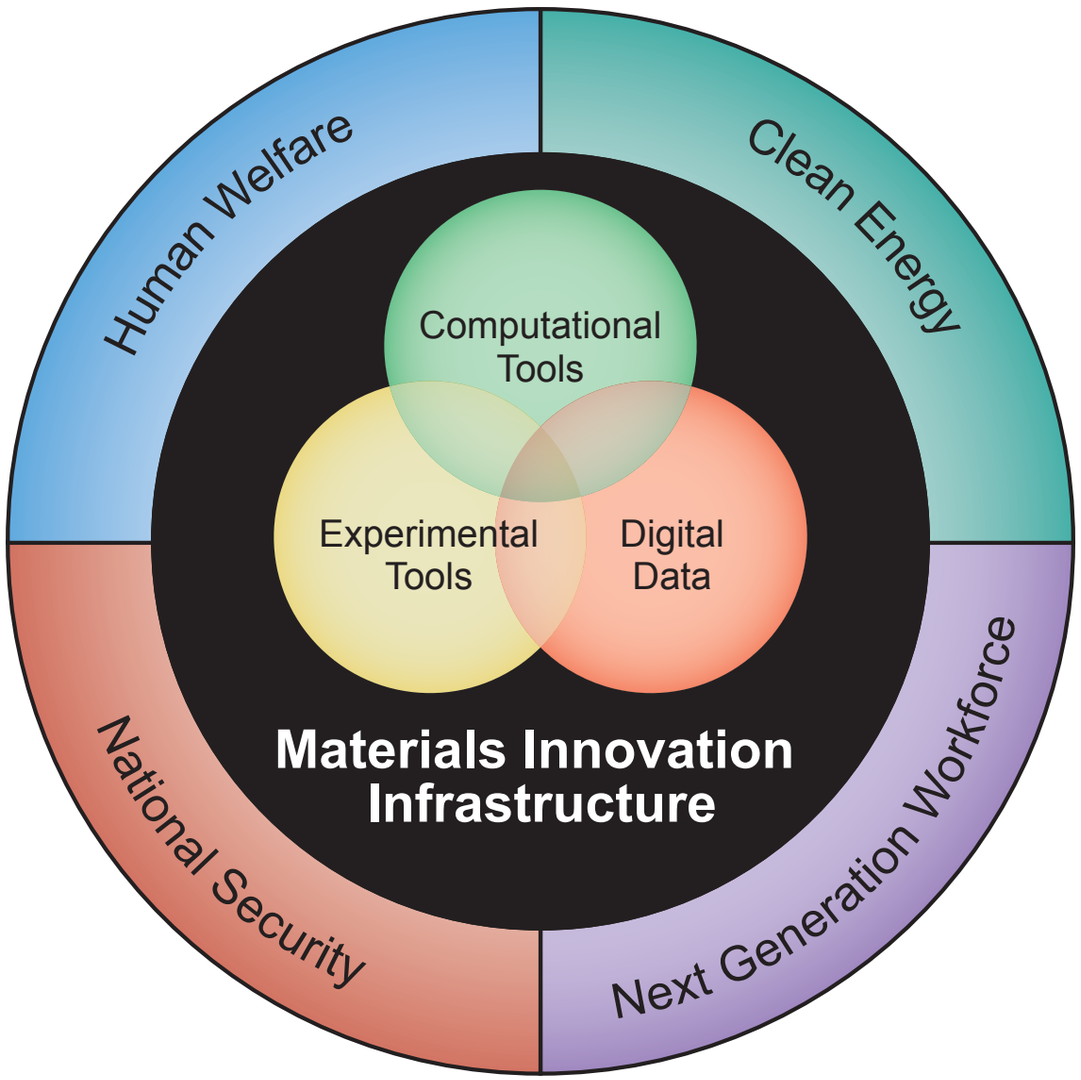


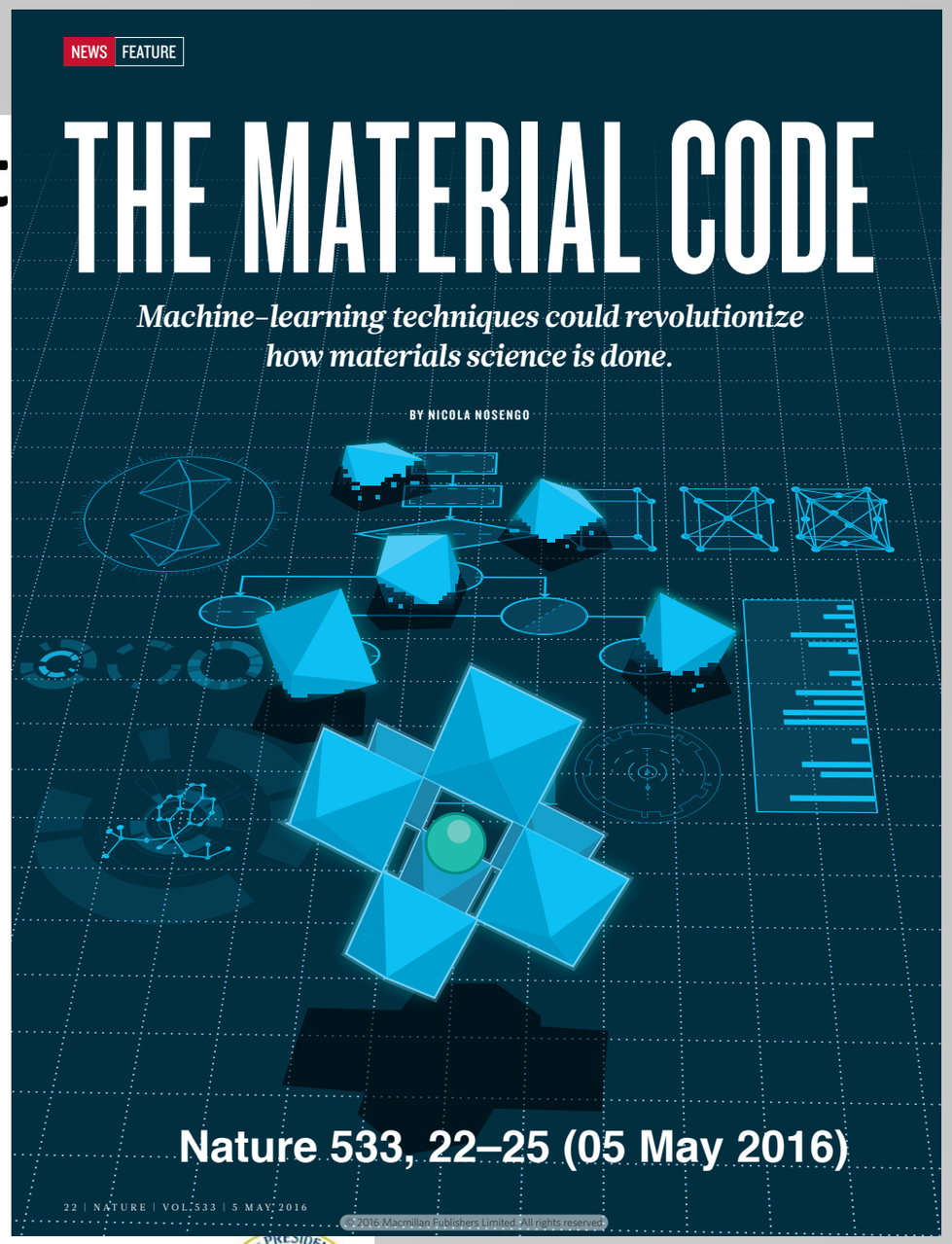


erc European Research Council

"To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call **the Materials Genome Initiative**.
The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. **We can do it faster.**"
-President Obama (6/11)

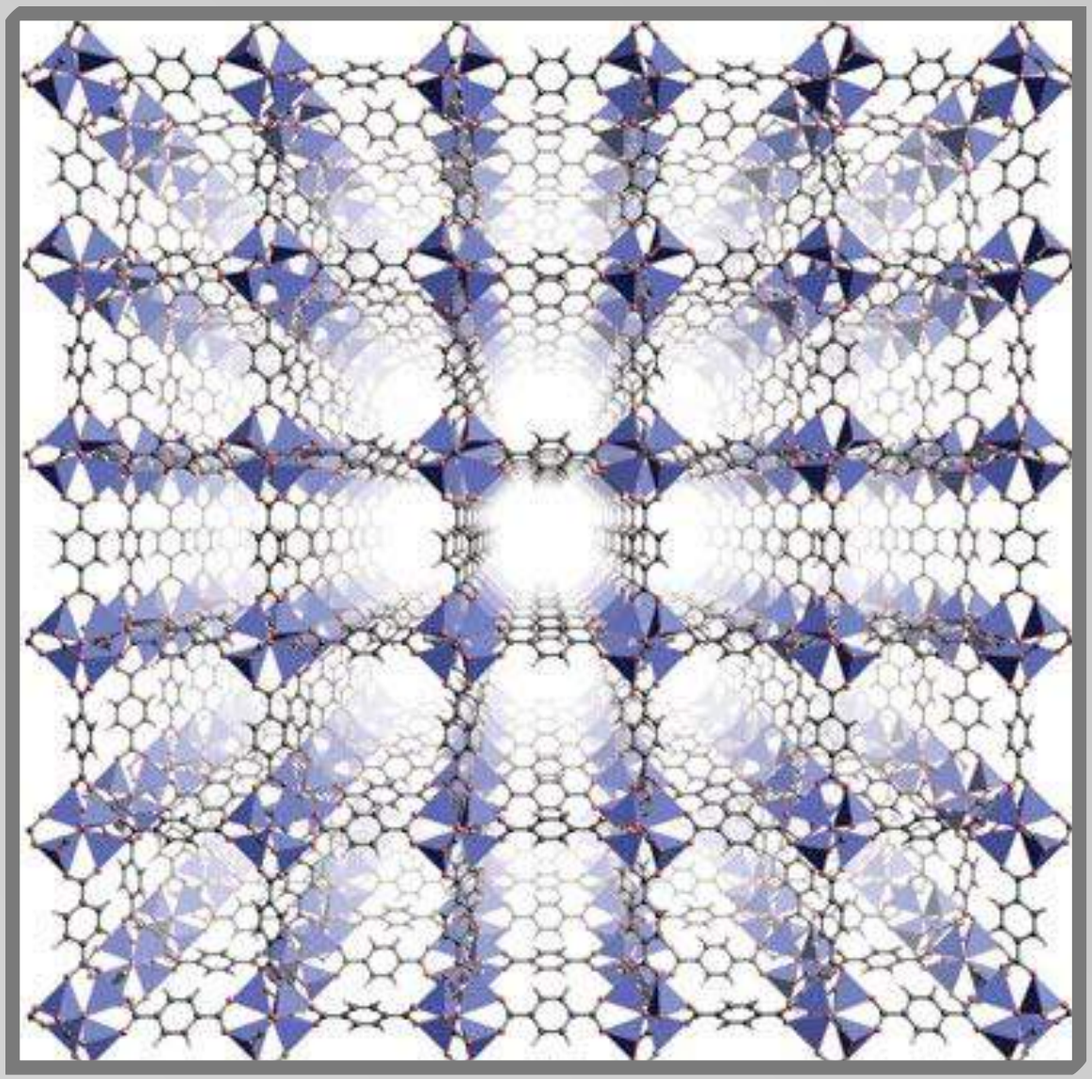
The Materials Innovation Infrast





http://www.whitehouse.gov/mgi

Metal Organic Frameworks



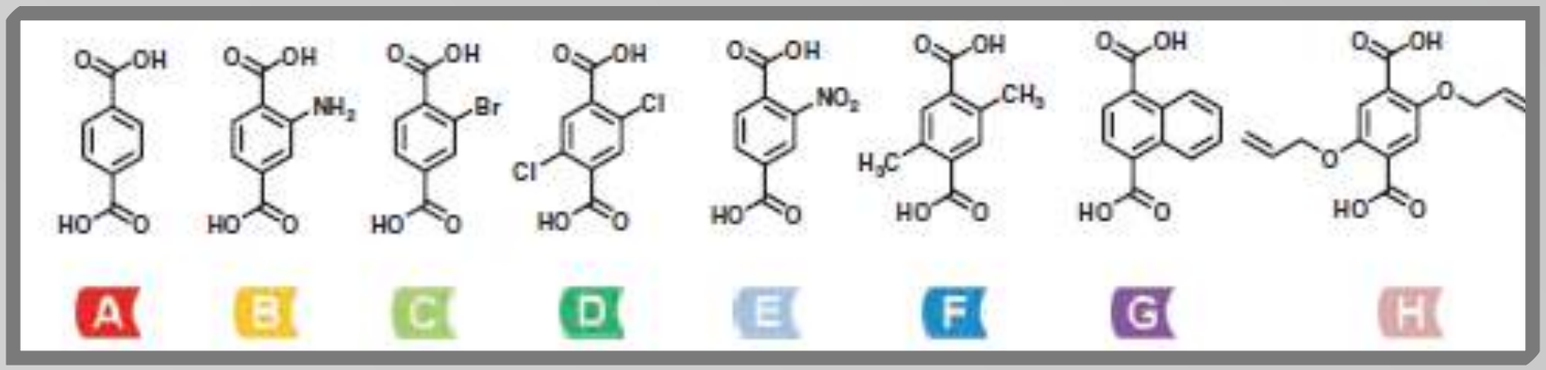
Zn_4O(1,4-benzenedicarboxylate)$_3$
MOF-5

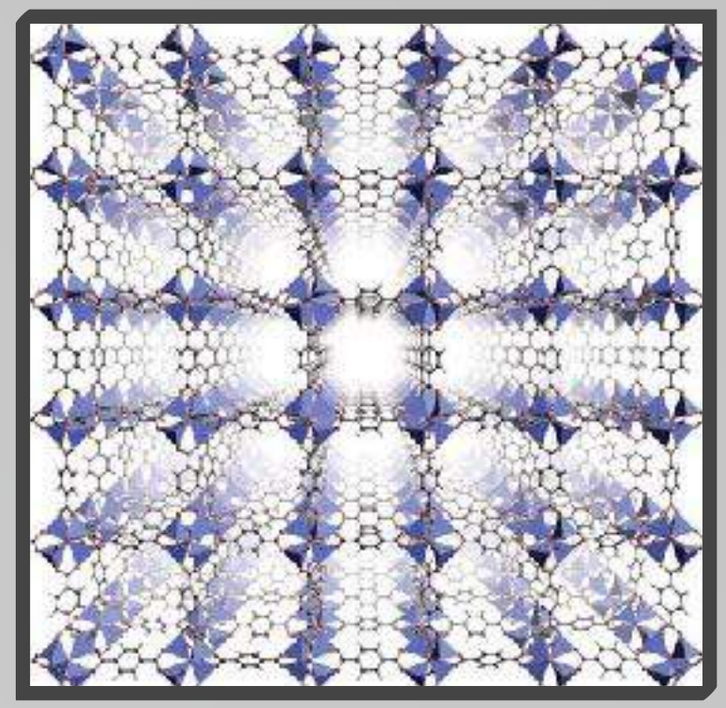
- BET surface areas up to 6200 m^2/g
- Density as low as 0.22 g/cm^3
- Tunable pore sizes up to 5 nm
- Channels connected in 1-, 2-, or 3-D
- Internal surface can be functionalized
- BASF production on ton scale

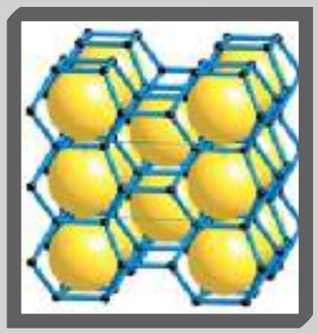
Computation Challenge

Chemical Flexibility of MOFs

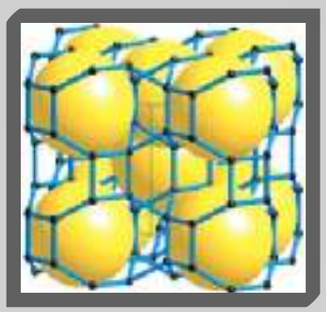
- We can change the metal: Fe, Mg, Ca, Zn, Cu, etc
- We can change the linker
- We can change the pore topology







crb



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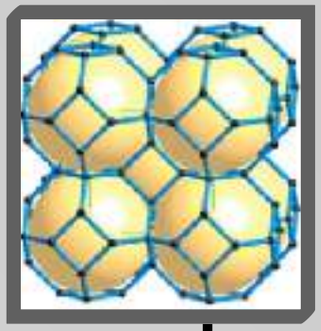
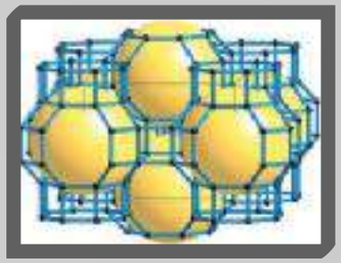


sod



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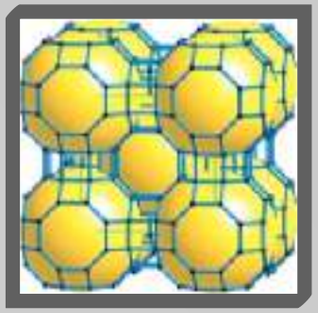
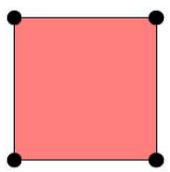
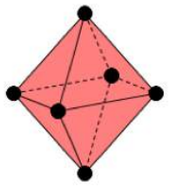
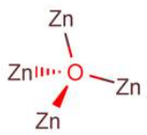
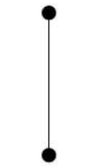
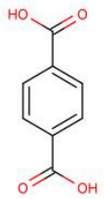
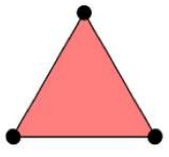
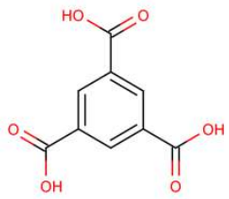
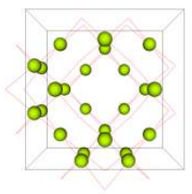
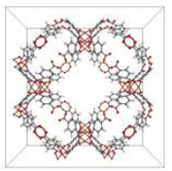
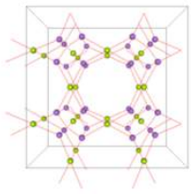
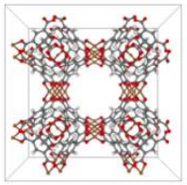
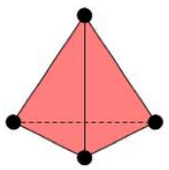
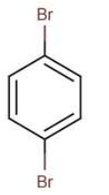
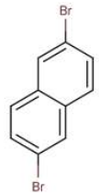
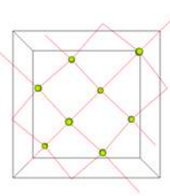
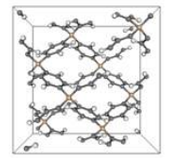
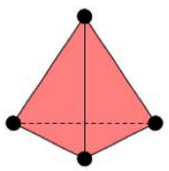
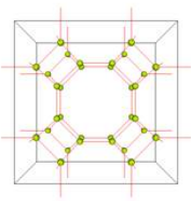
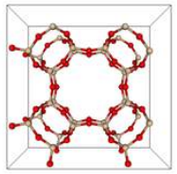
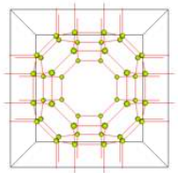
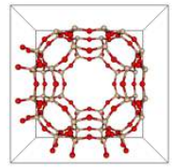
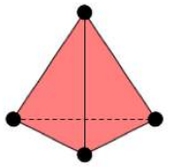
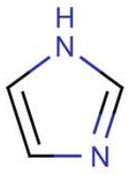
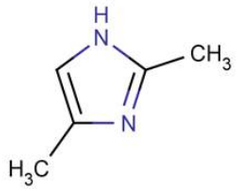
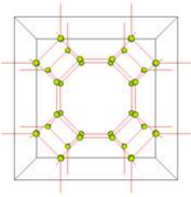
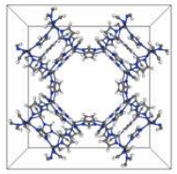
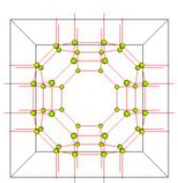
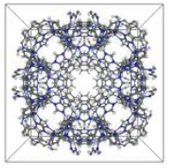


rho

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

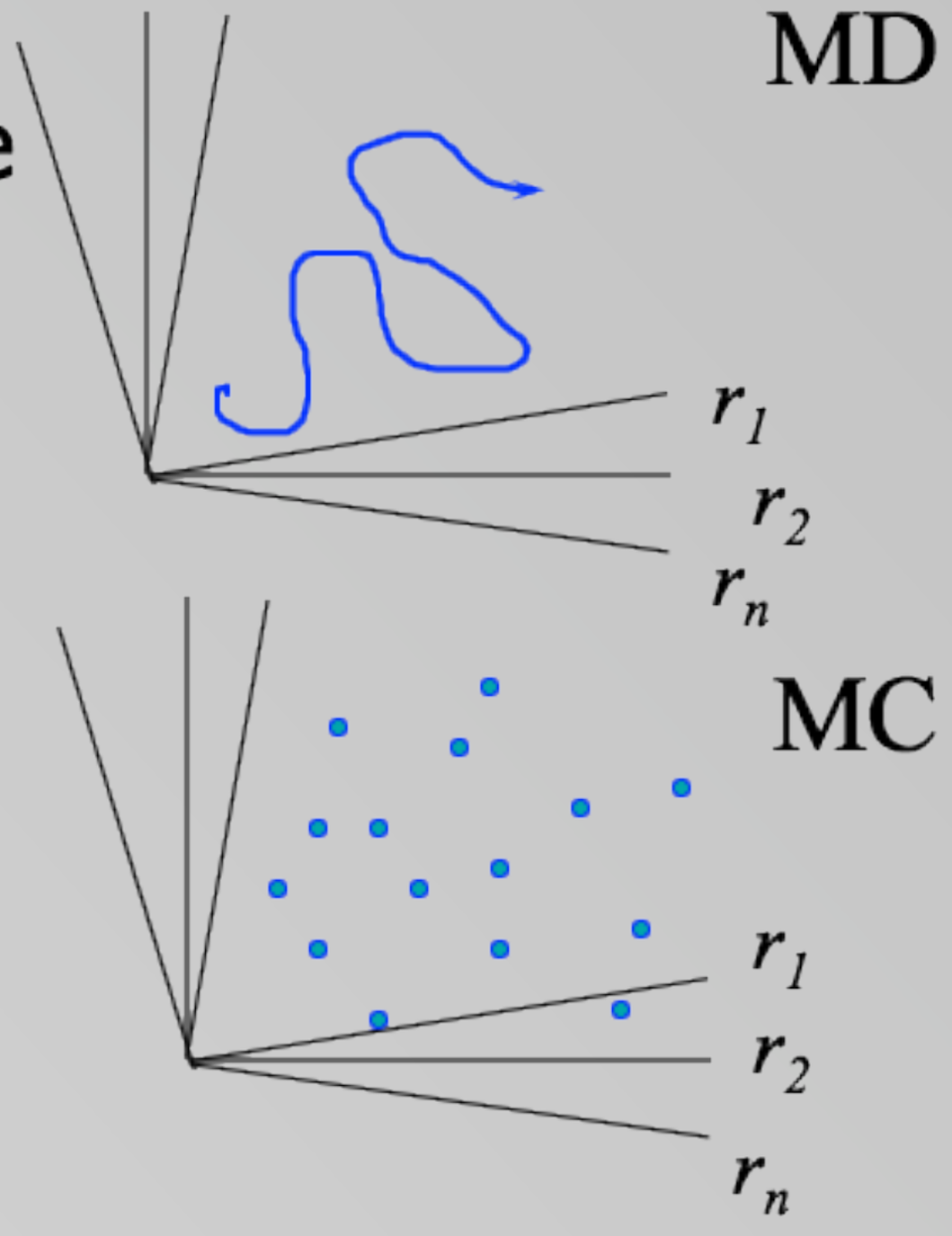
Material class	Building blocks				Topologies	
MOFs	 Cu—Cu	 	 	 	 	 
PPNs	 Si Ge				 	
Zeolites	 Si		O		 	 
ZIFs	 Zn Fe				 	 

> 3,000,000 materials

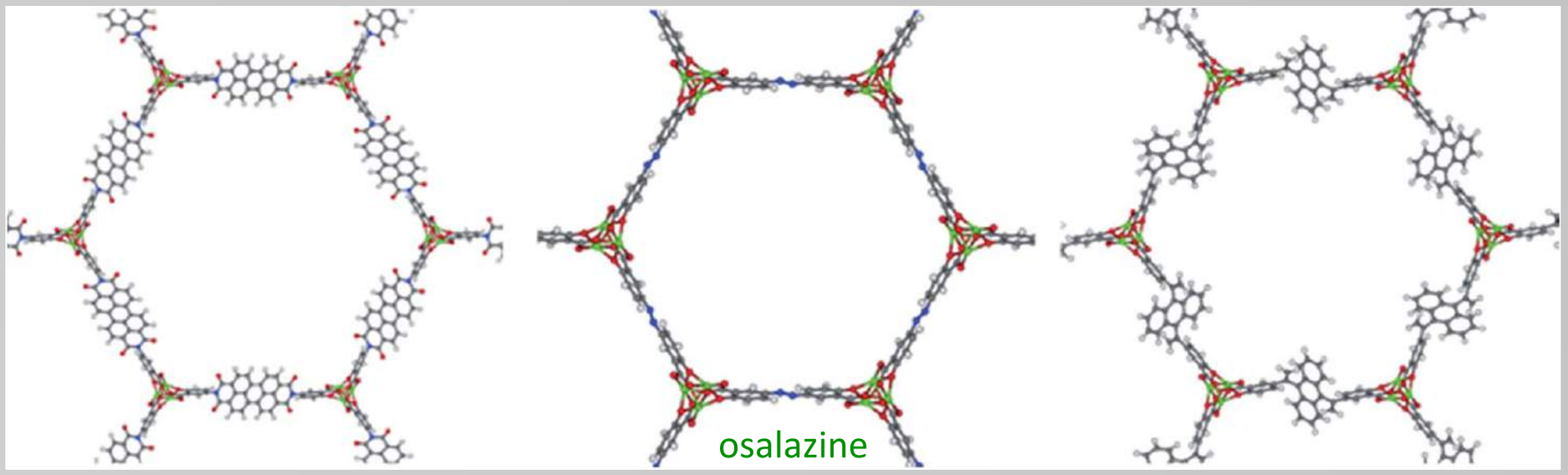
Molecular Simulations

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

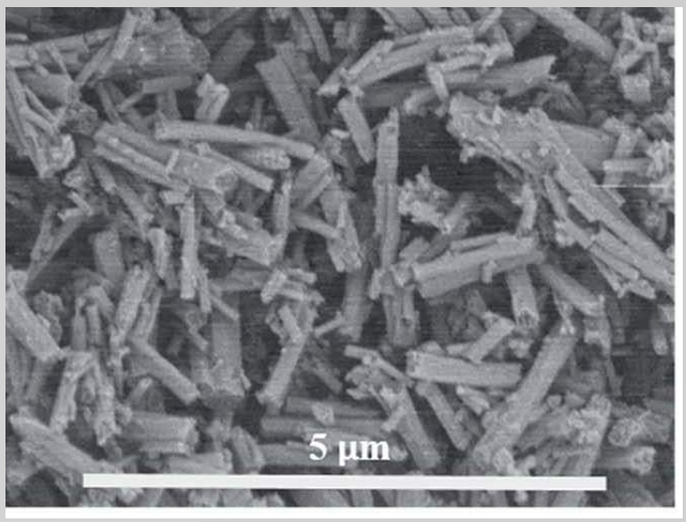
- calculate thermodynamic and transport properties for a given intermolecular potential

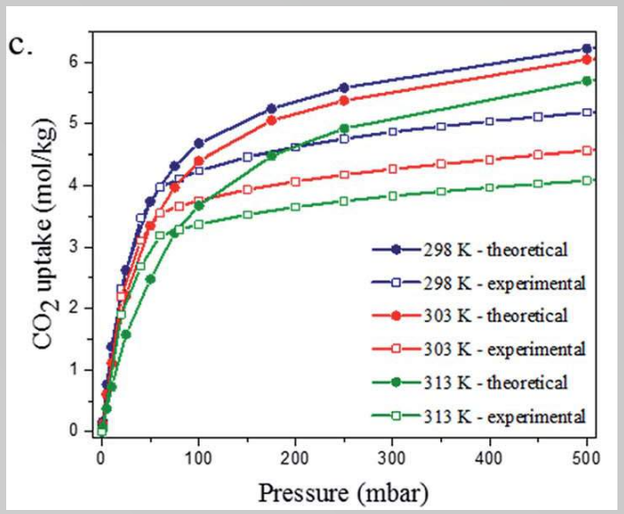


Can we predict the performance of a material before its synthesis?



We predicted the structure of Mg_2(osalazine) and subsequent synthesis confirmed the predicted structure and adsorption properties





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

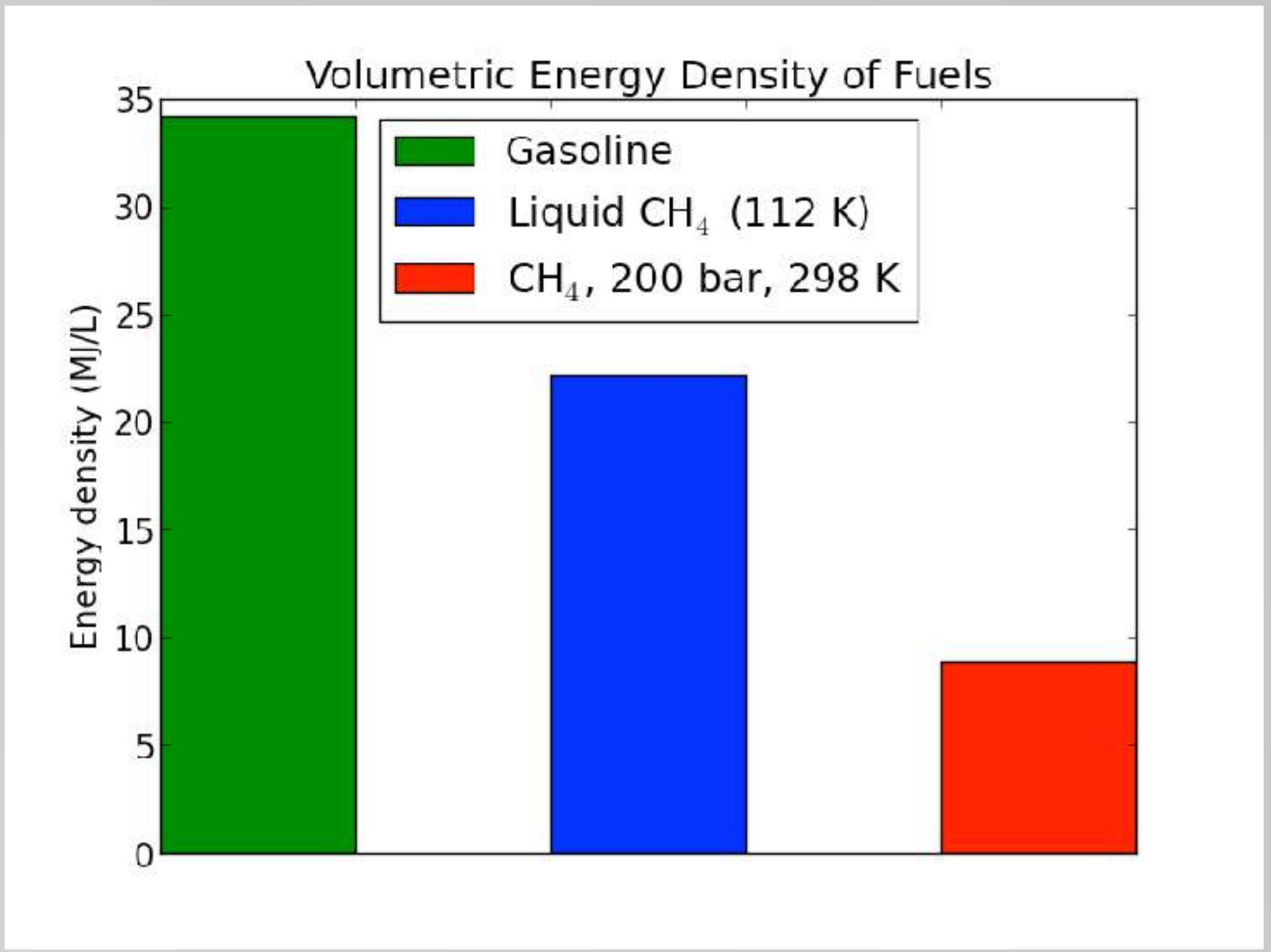
Methane Storage

Methane cars: the technological obstacle

0.036 MJ

34.2 MJ

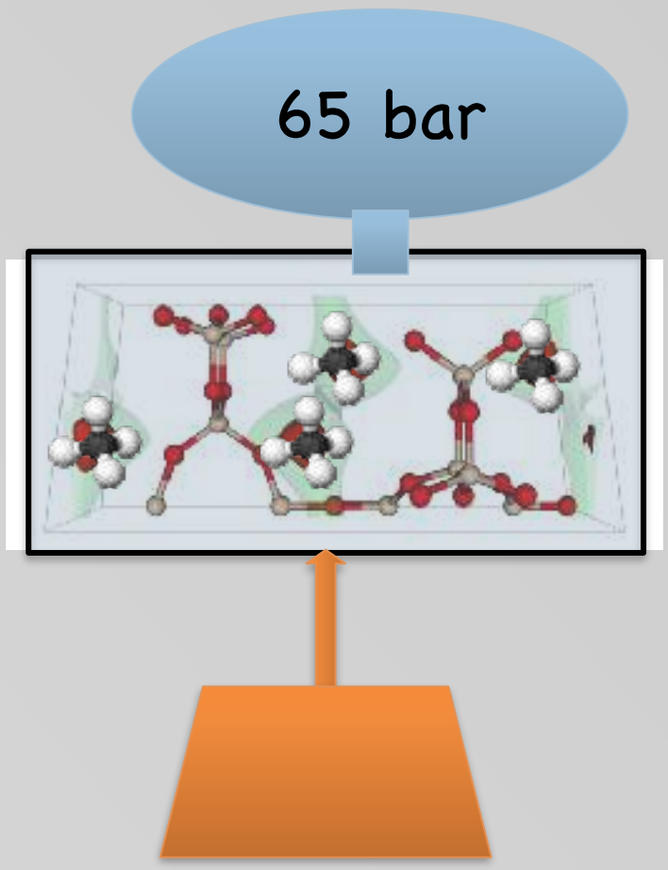
Methane versus gasoline



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

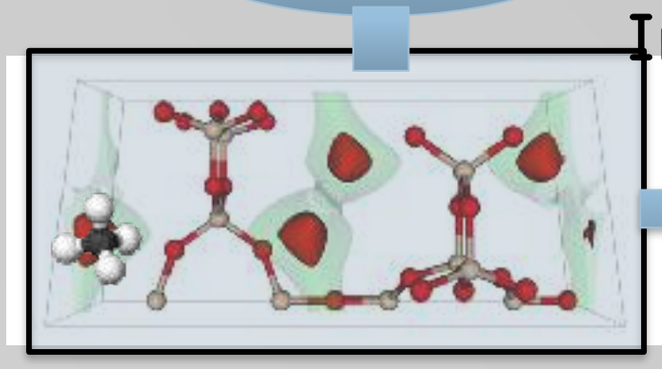
Can we find a material with the same energy density as compressed natural gas?

65 bar



P_H = 65 bar

5.8 bar

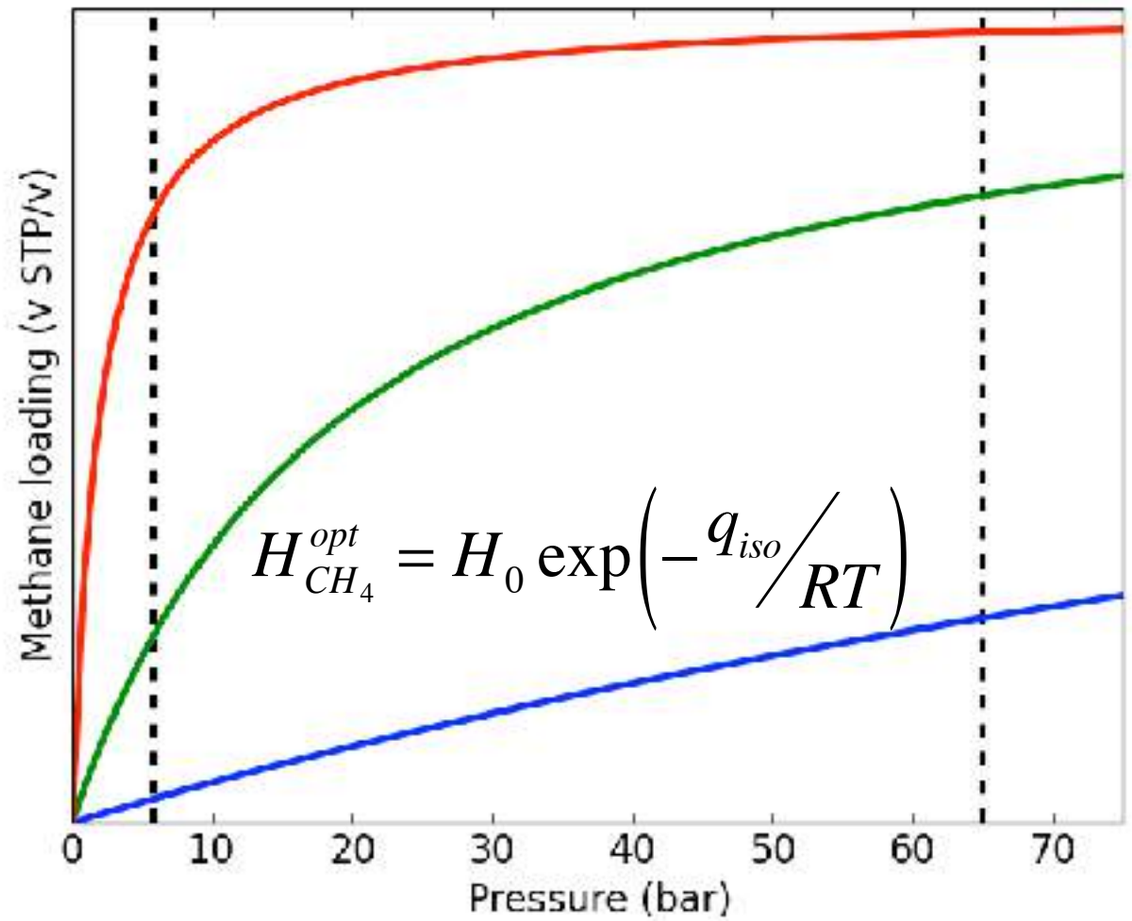


Insufficient flow

~1 bar

P_L = 5.8 bar

Goal: maximize deliverable capacity



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

Langmuir 2006, *22*, 1688−1700

Optimum Conditions for Adsorptive Storage

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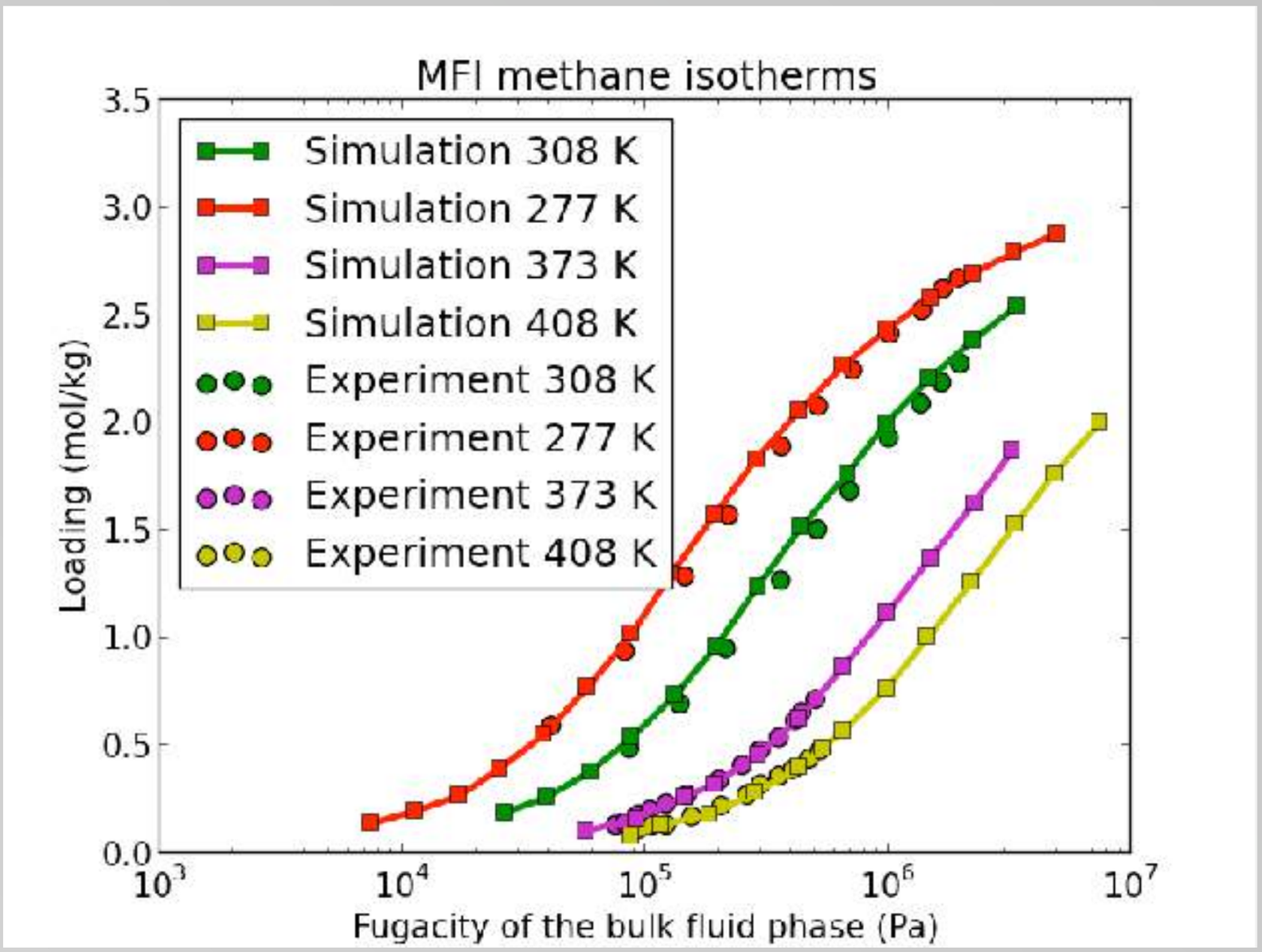
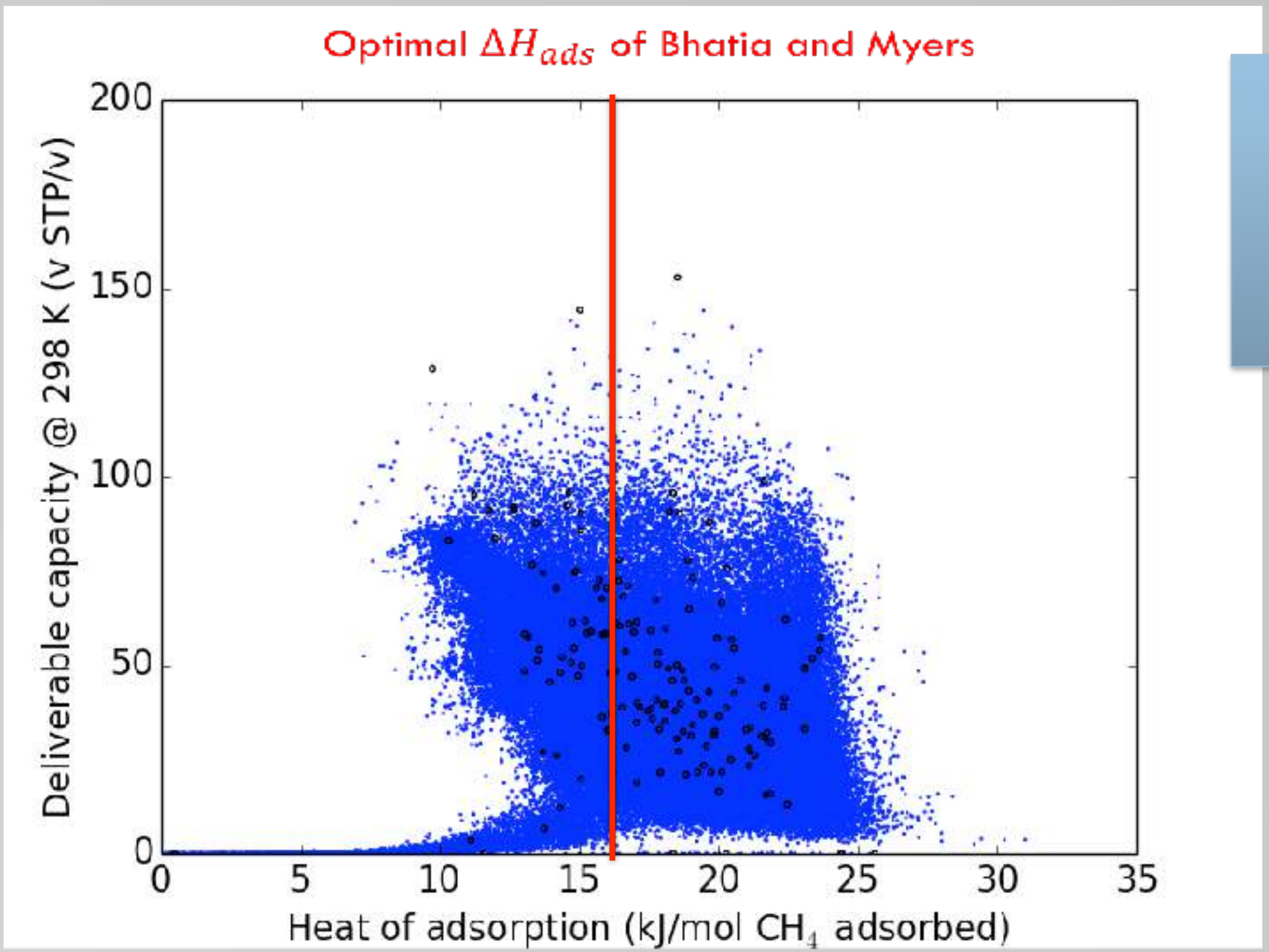
… but only a limited number of materials were analyzed

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



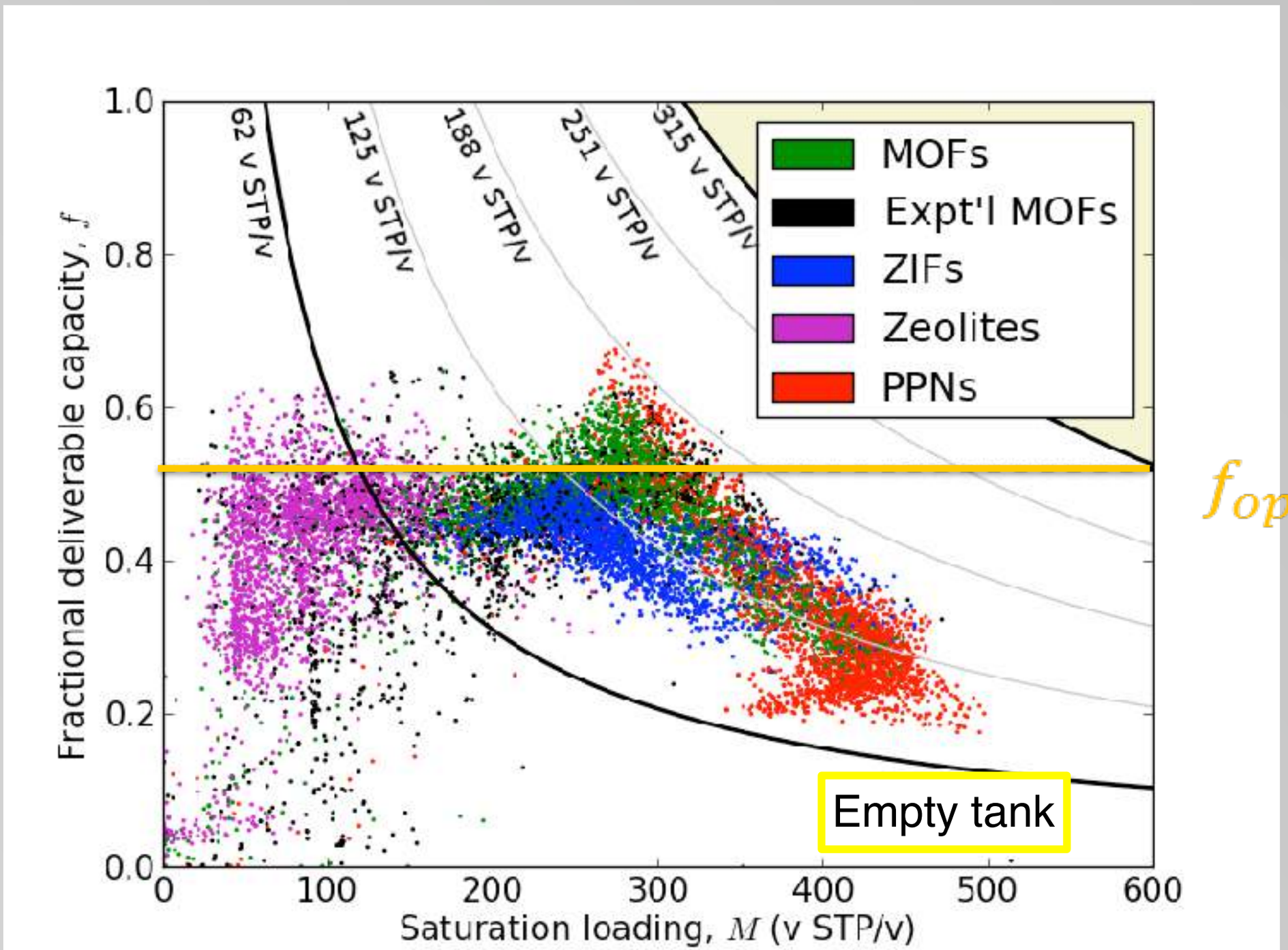
C. Simon *et al*. (2014) *Phys. Chem. Chem. Phys*. 16 (12), 5499-5513

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

Methane storage in all silica zeolites:

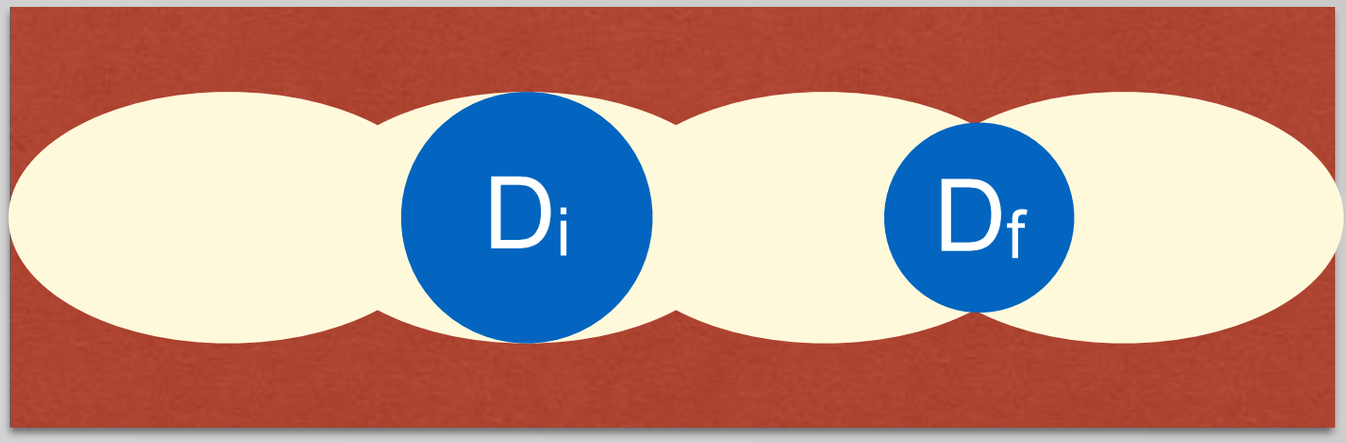
- only the pore shape matters
- similar pores should have similar performance

How to compare pores?

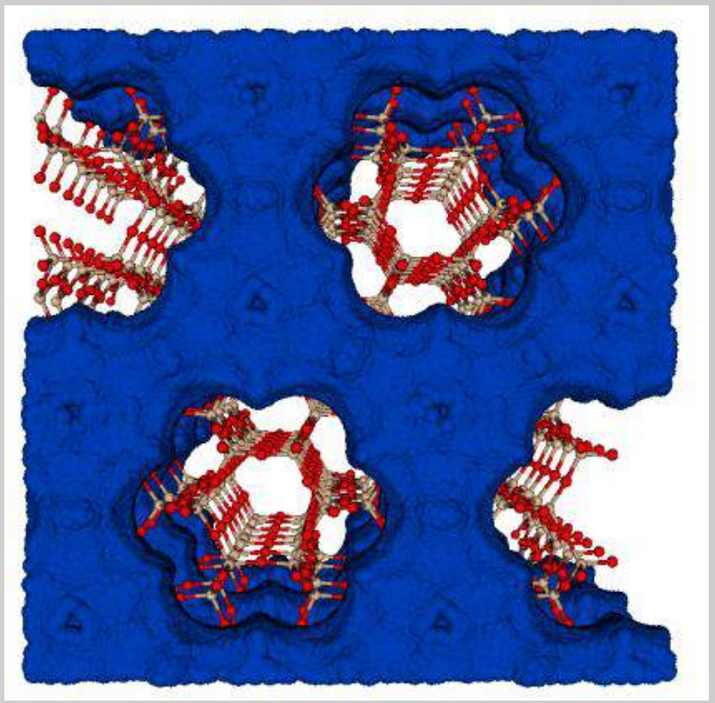
Simple Descriptors

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

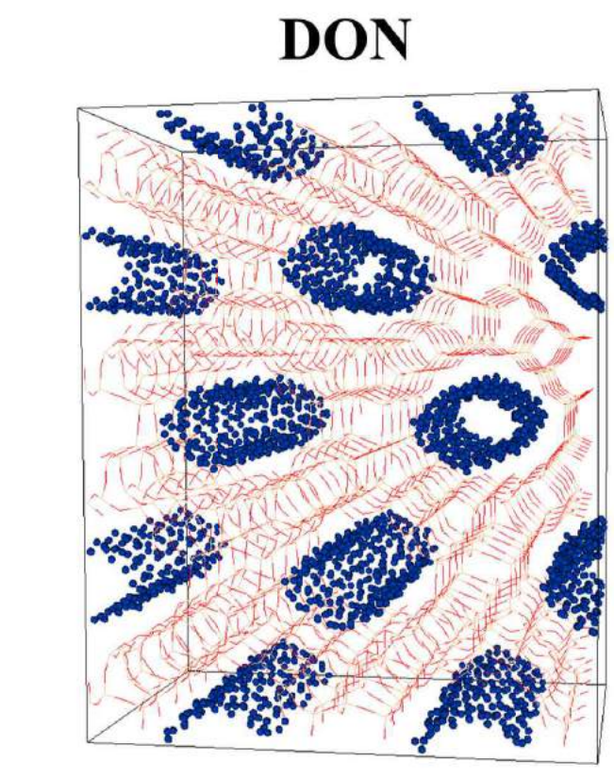


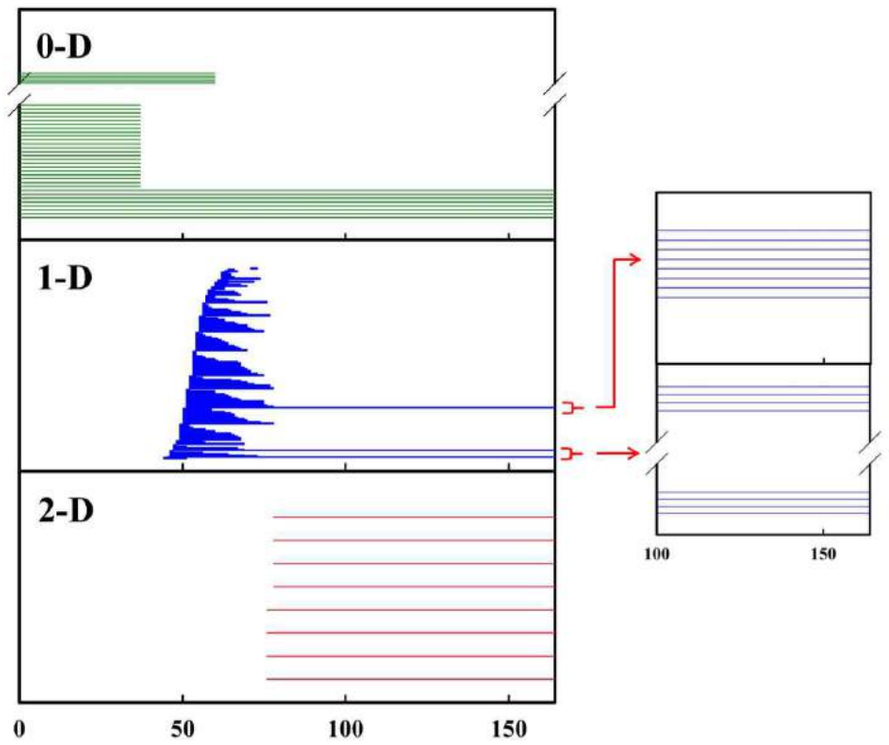
SSF

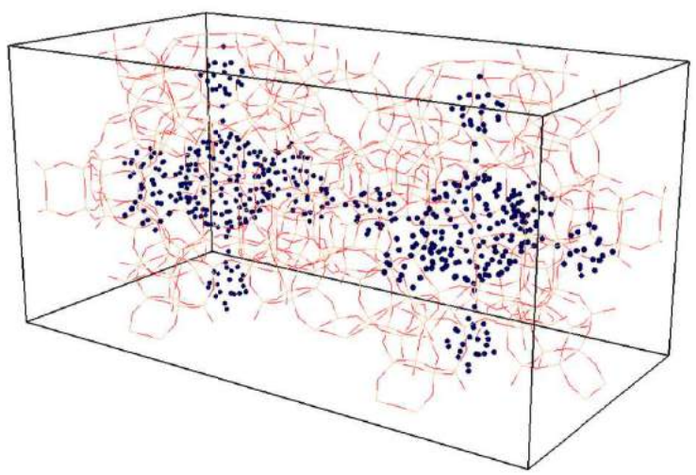


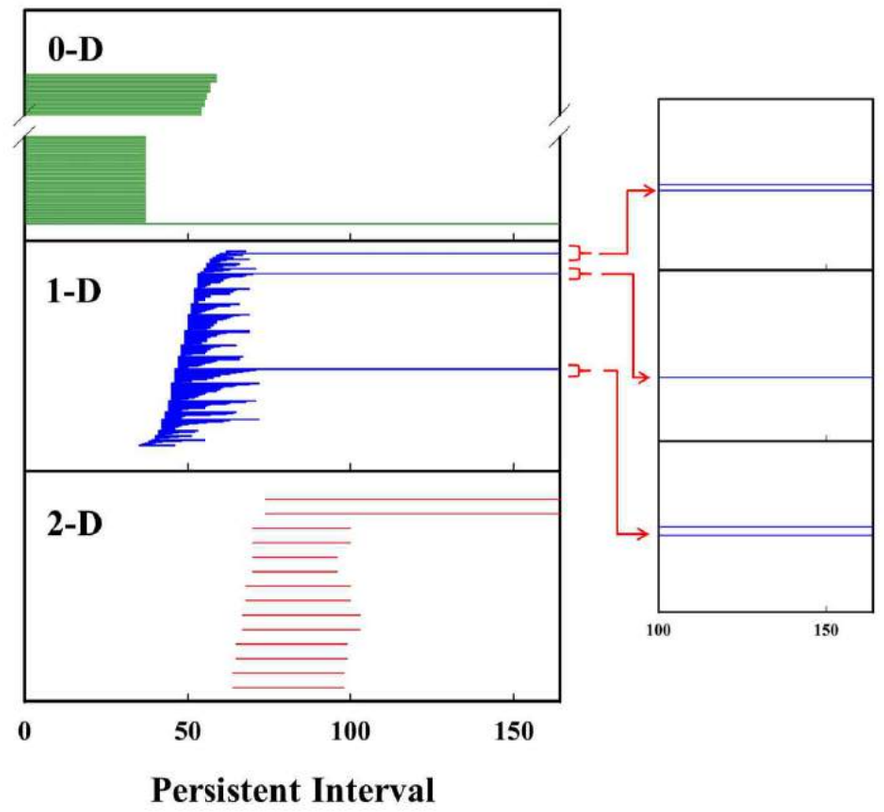
		name	D_i	D_f	ρ	ASA	AV
CD	Seed	SSF	7.59	6.15	1.64	1191	0.122
	1st	h8242590	7.87	6.16	1.62	1210	0.119
	2nd	h8239380	7.60	6.29	1.63	1156	0.120
	3rd	h8267258	7.72	6.21	1.63	1205	0.115
	4th	h8070132	7.69	6.49	1.62	1187	0.126

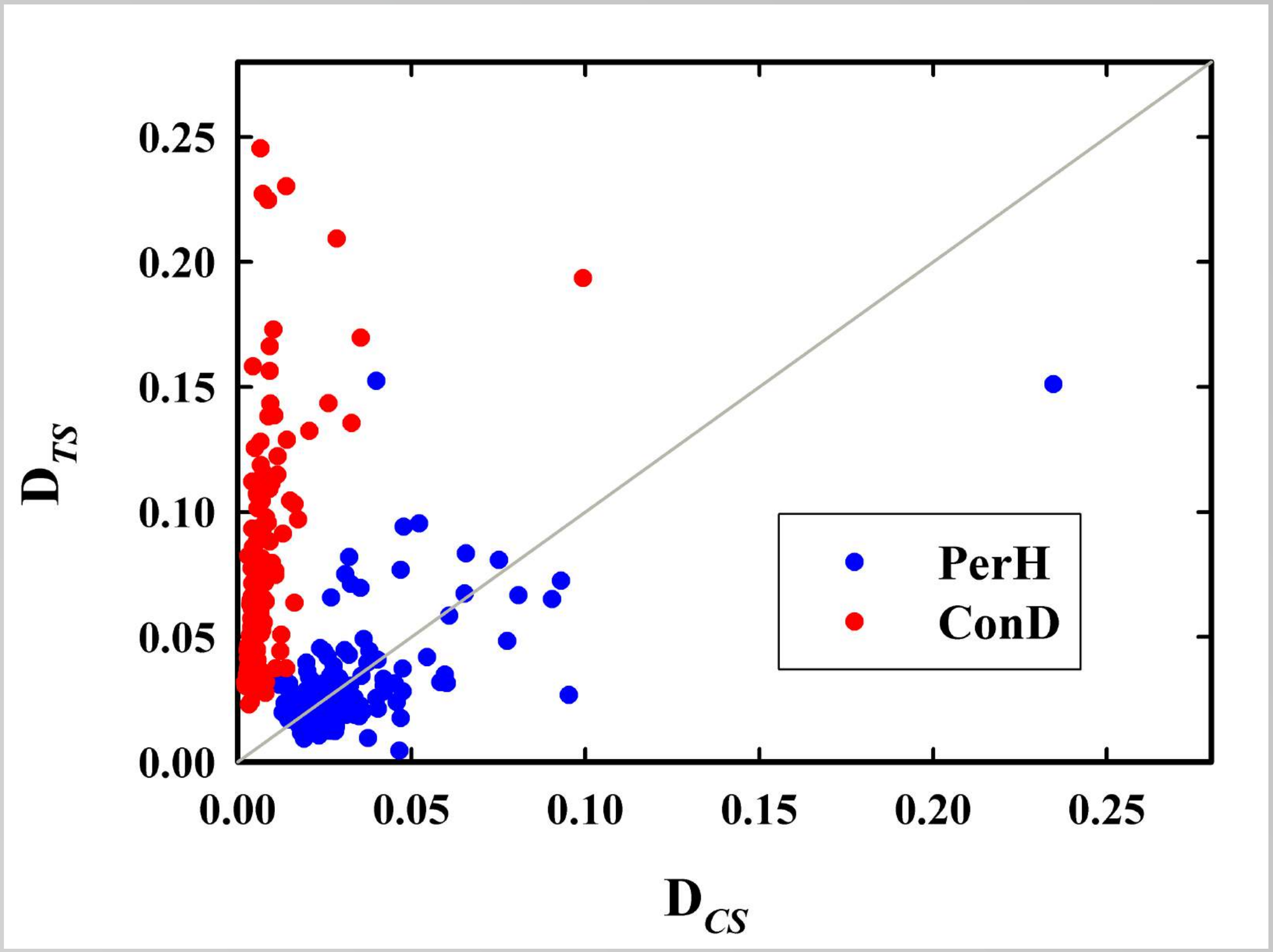
Persistent Homology

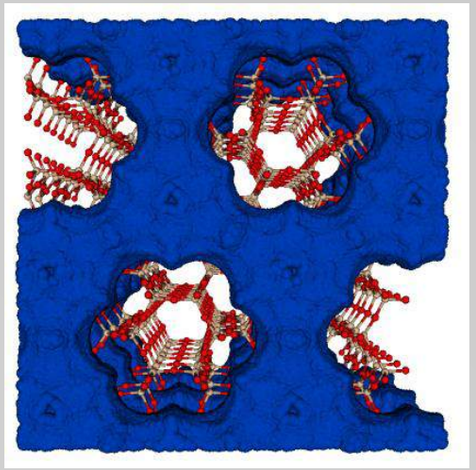
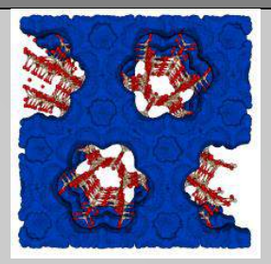
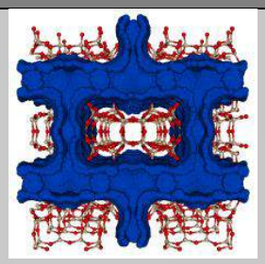
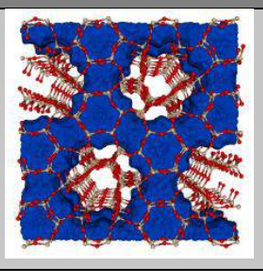
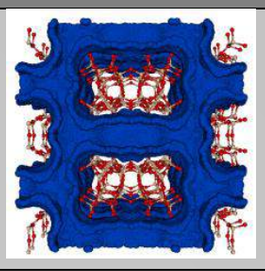
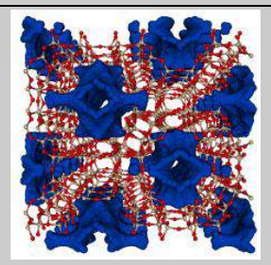
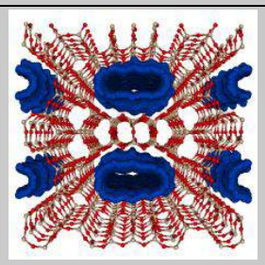
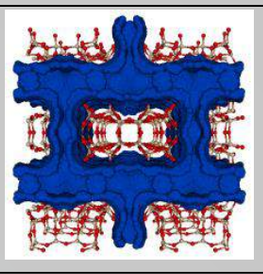
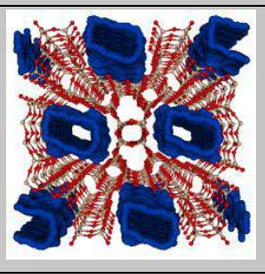
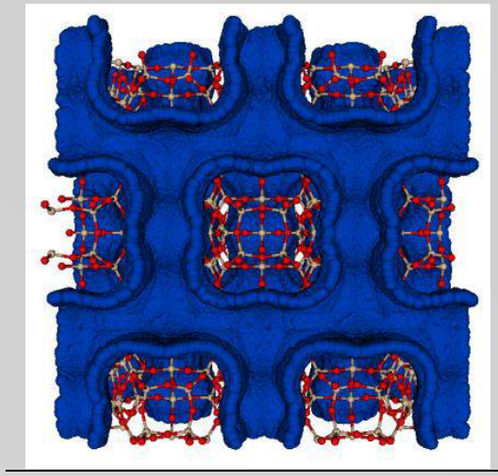
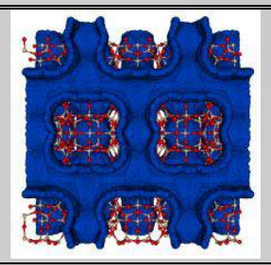
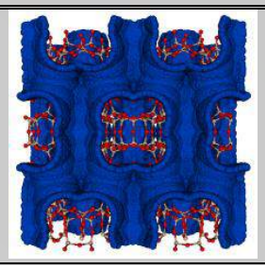
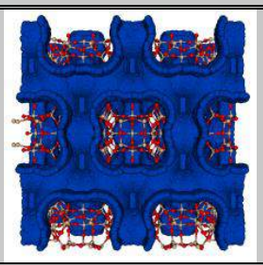
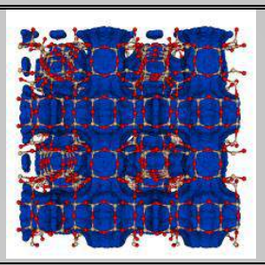
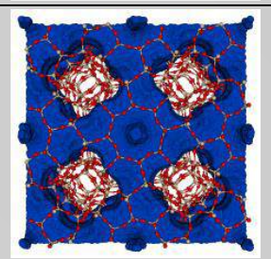
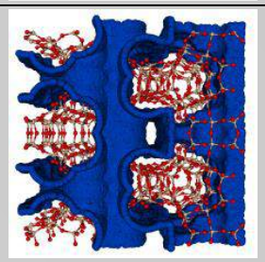
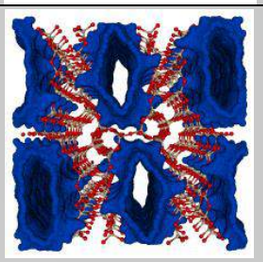
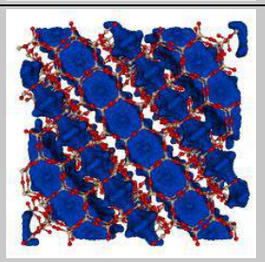


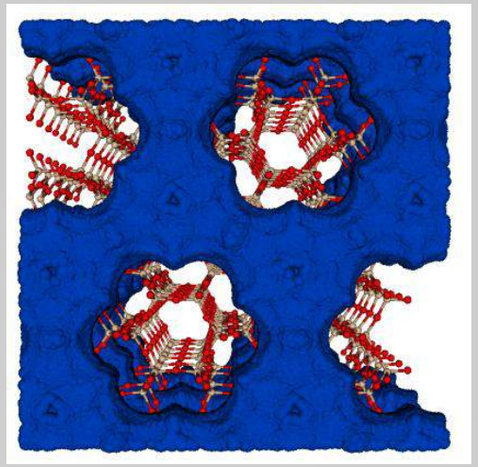
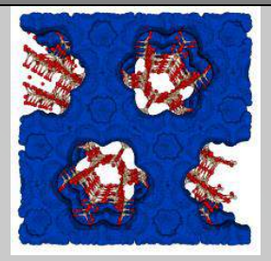
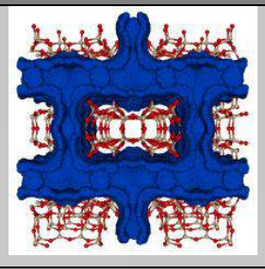
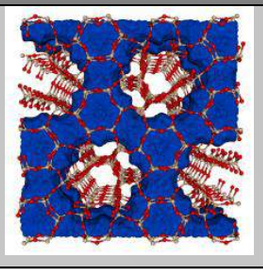
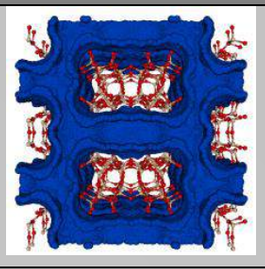
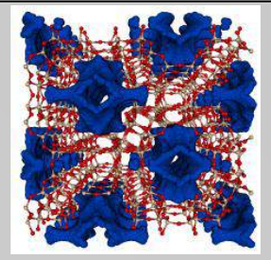
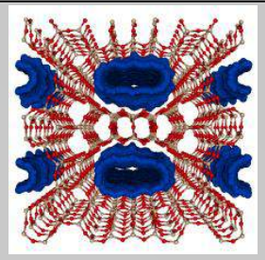
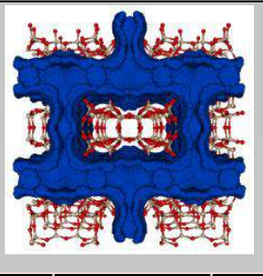
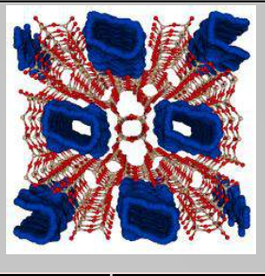






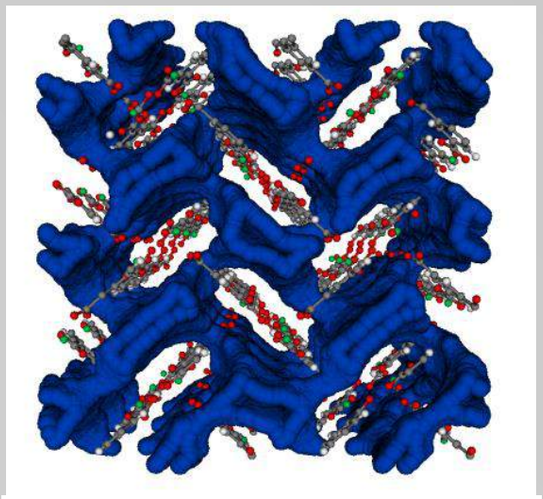

0.25
0.20
0.15
0.10
0.05
0.00
D_{TS}
0.00
0.05
0.10
0.15
0.20
0.25
D_{CS}
PerH
ConD

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

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

AFUPEX



Gaodeng Xuexiao Huaxue Xuebao, 2007, 28, 1437

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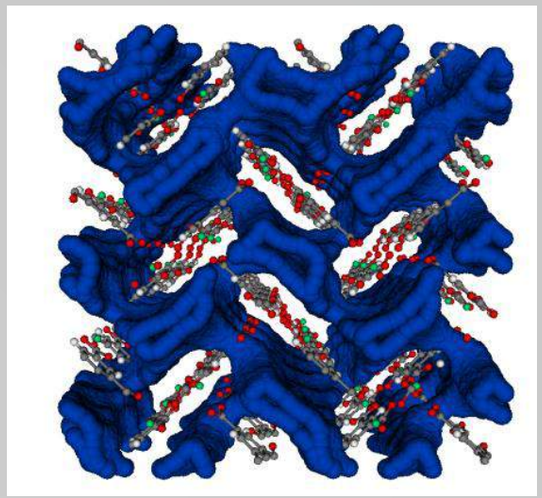

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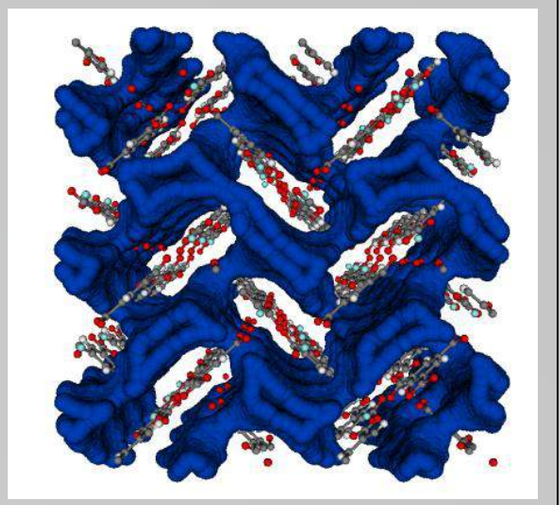

Inorg. Chem. 45, 4065 (2006)

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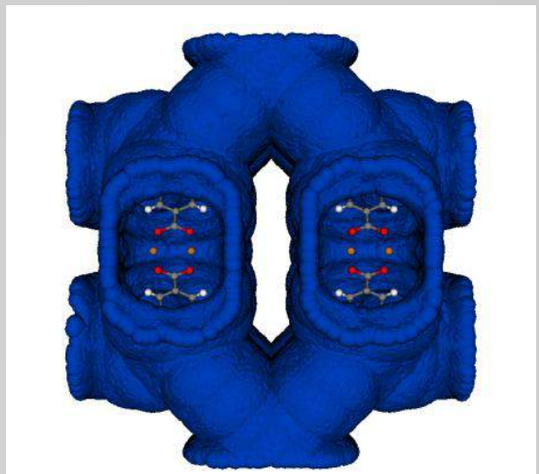

Inorg. Chem. 50, 9147 (2011)

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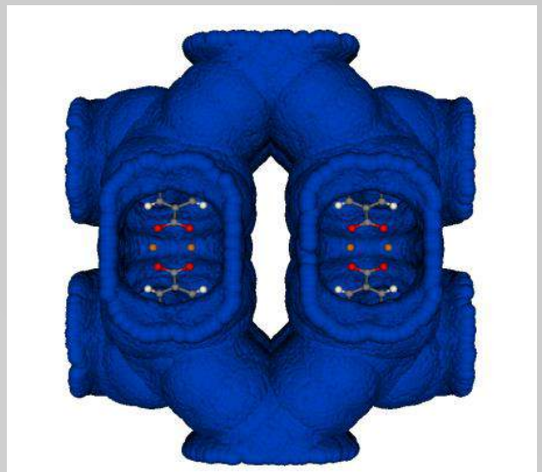

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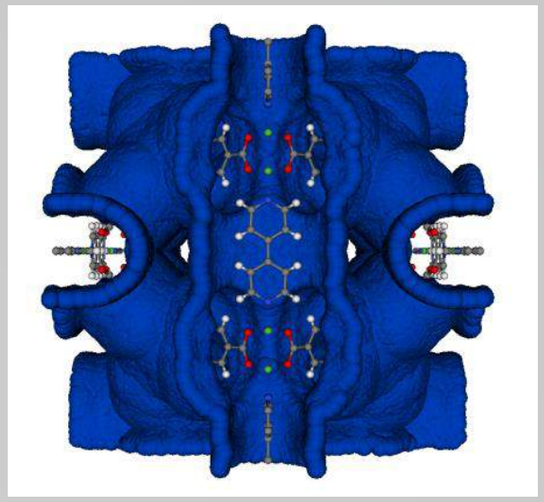
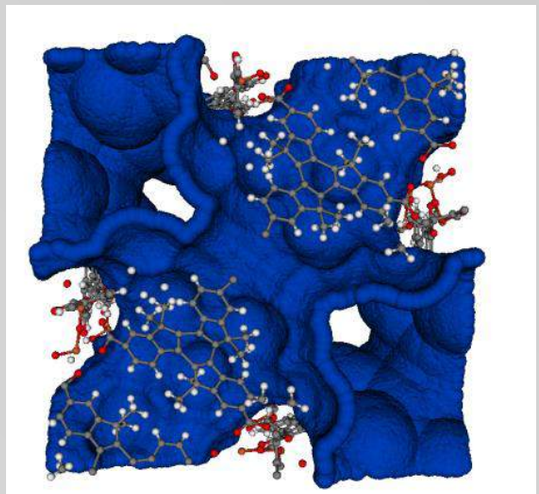


Chem. Eur. J. 17, 13007 (2011)

VETTIZ



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

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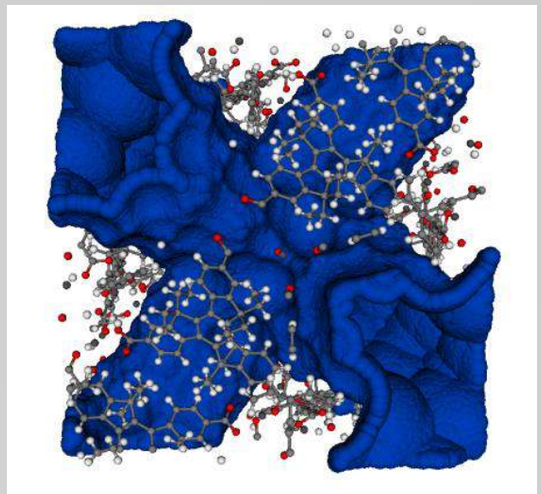

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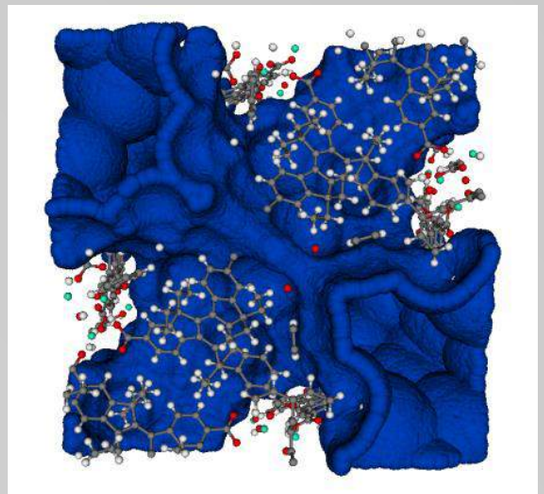
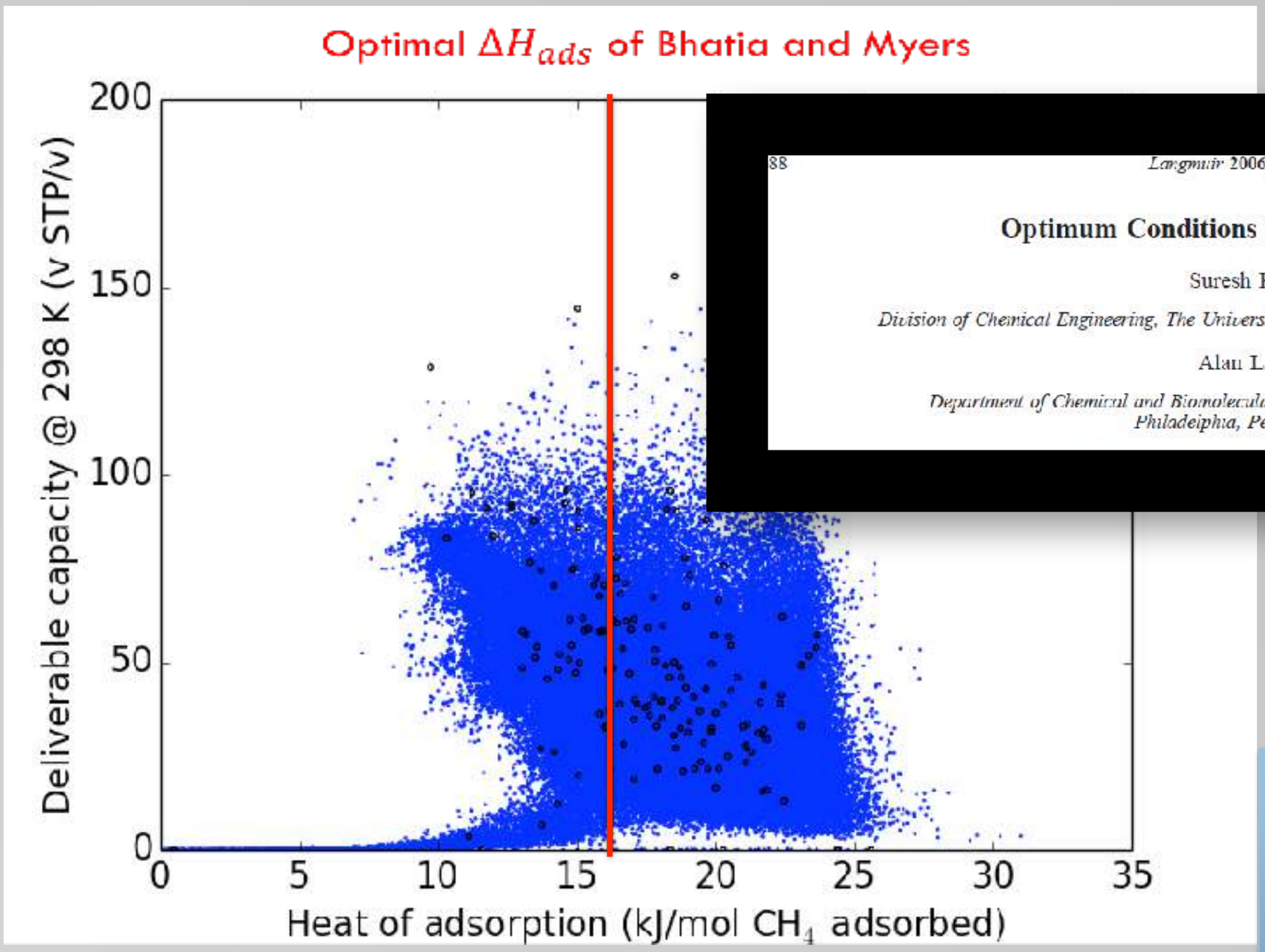


J. Am. Chem. Soc. 131, 3814 (2009)

180 known zeolites
>10,000 MOFs

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

In silico screening of zeolites



88 *Langmuir* 2006, *22*, 1688−1700

Optimum Conditions for Adsorptive Storage

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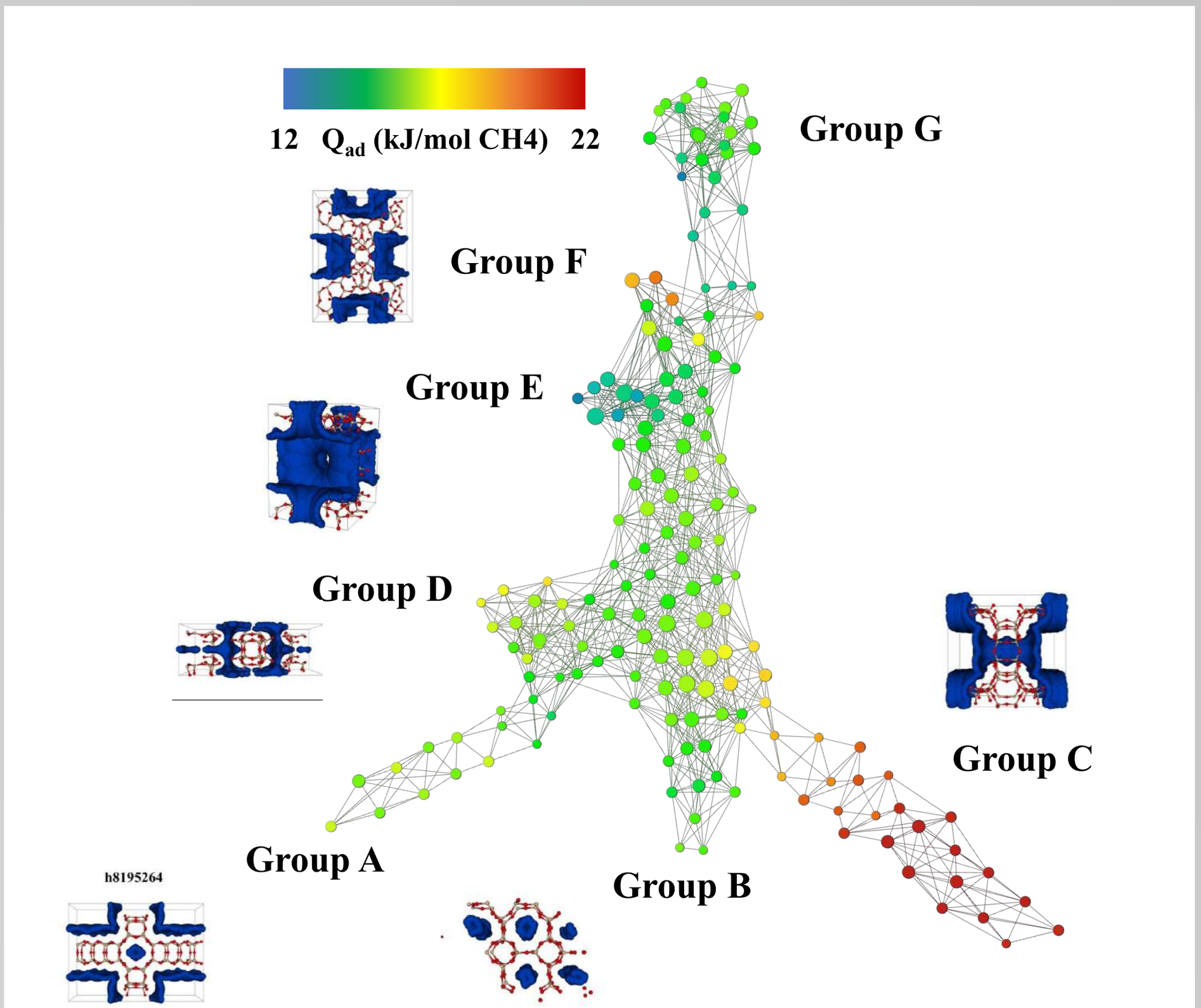
Alan L. Myers*

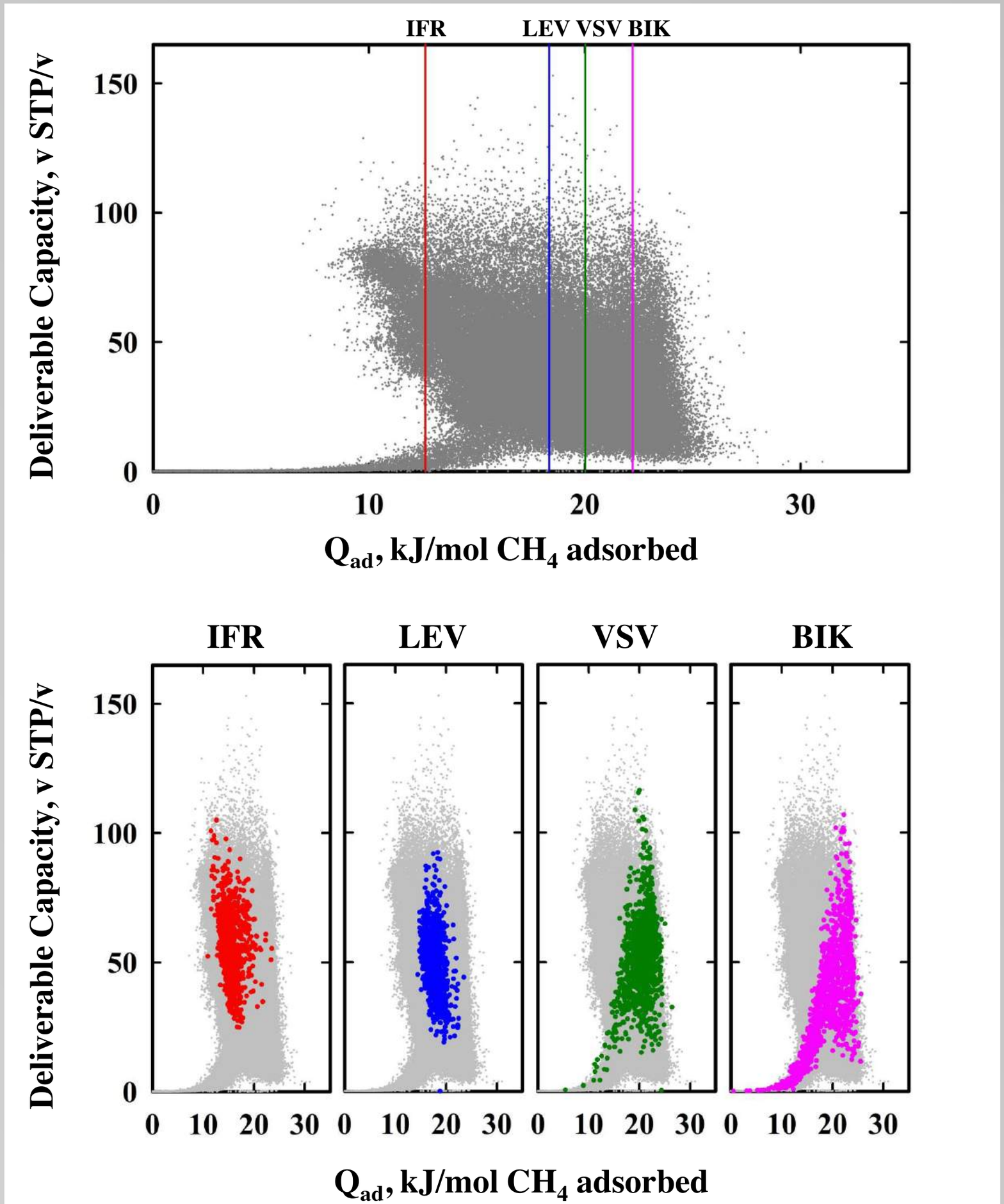
Department of Chemical and Biomolecular Engineering, University of Pennsylvania Philadelphia, Pennsylvania 19104

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

Heat of a adsorption of top performing materials

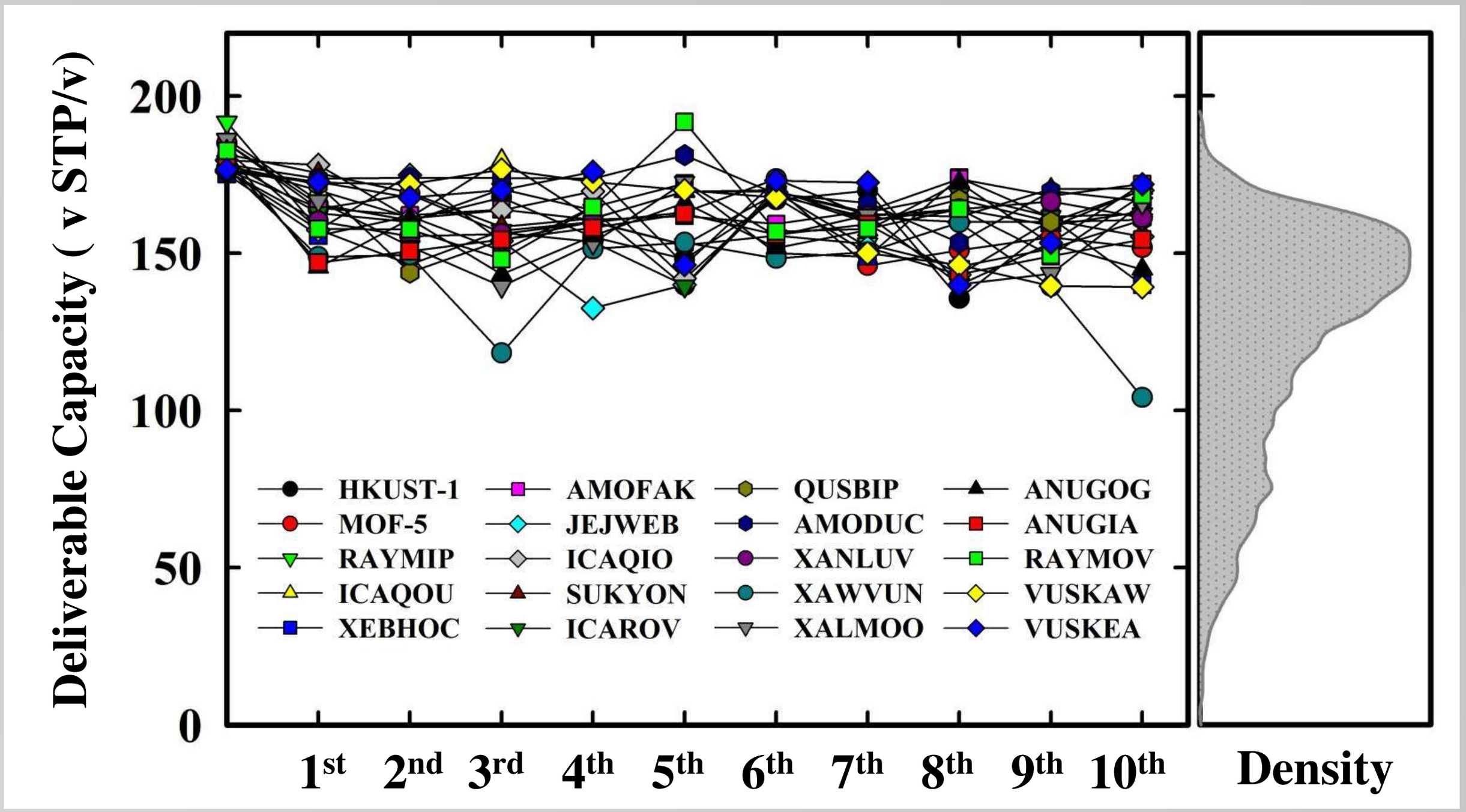


Y. Lee, et al. Nat. Commun. **8** (2017) http://dx.doi.org/10.1038/ncomms15396



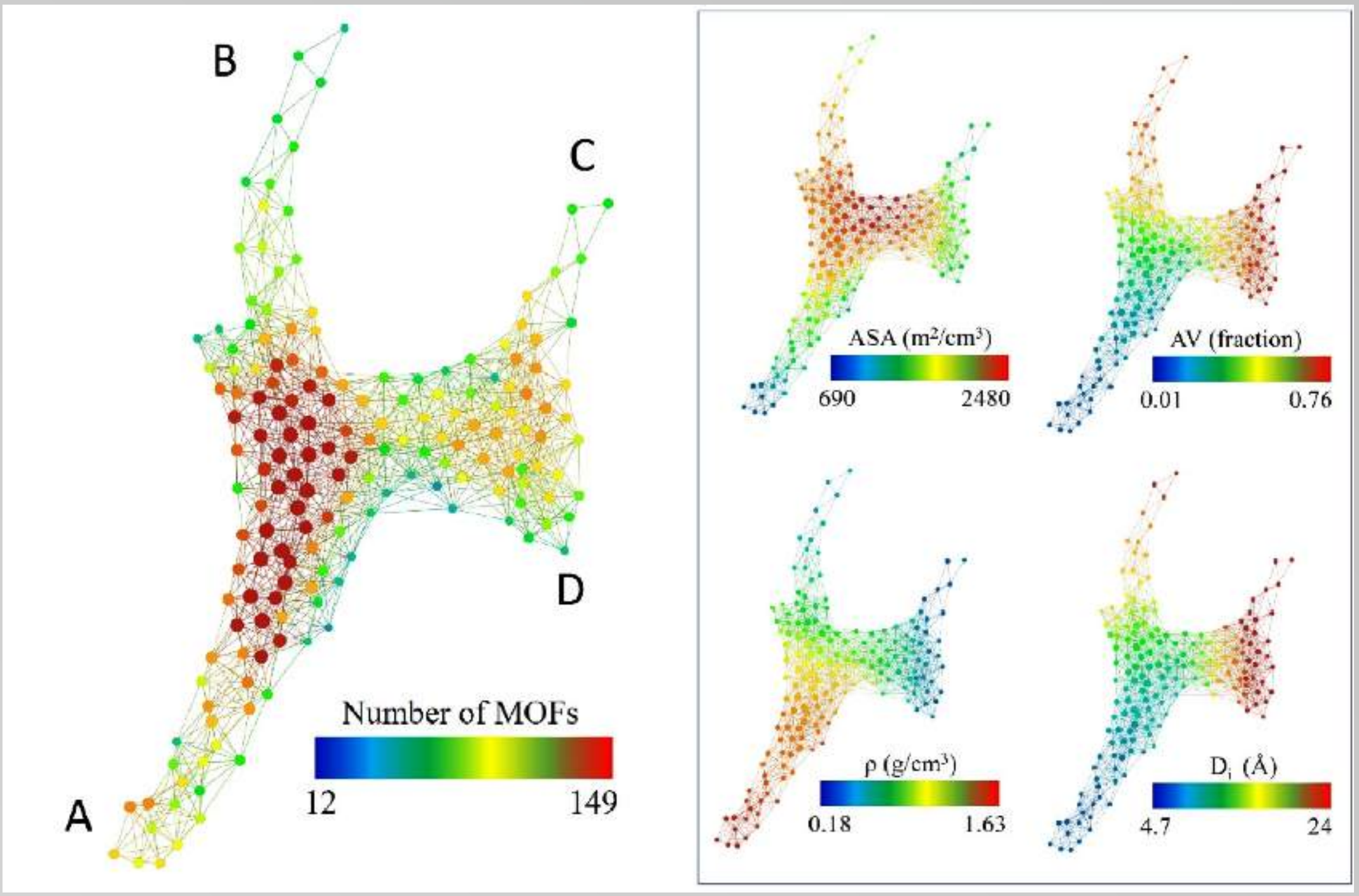
Y. Lee, et al. Nat. Commun. **8** (2017) http://dx.doi.org/10.1038/ncomms15396

Similar materials have similar performance



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

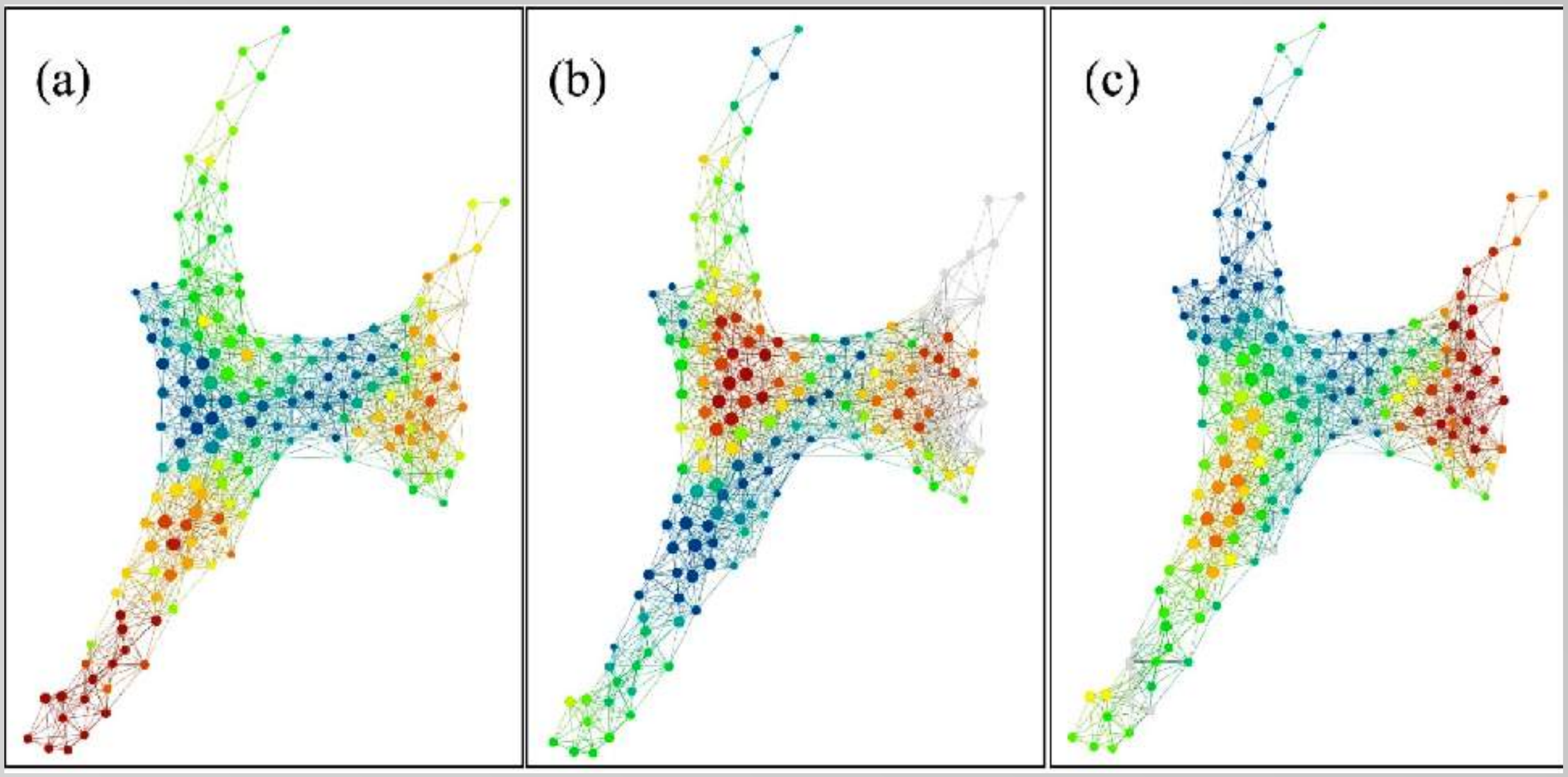
Diversity of MOF Materials Database



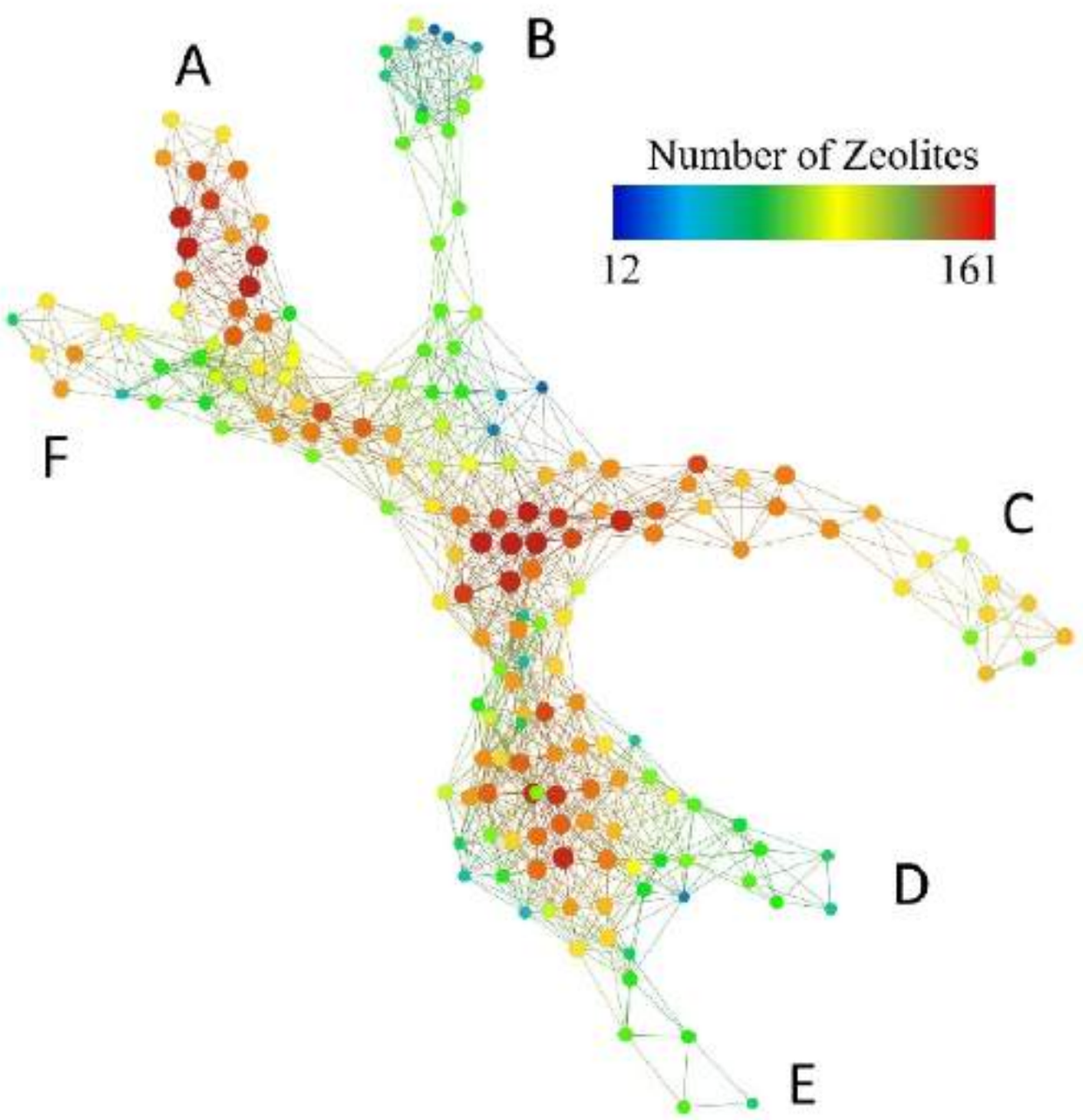
Five Different Types

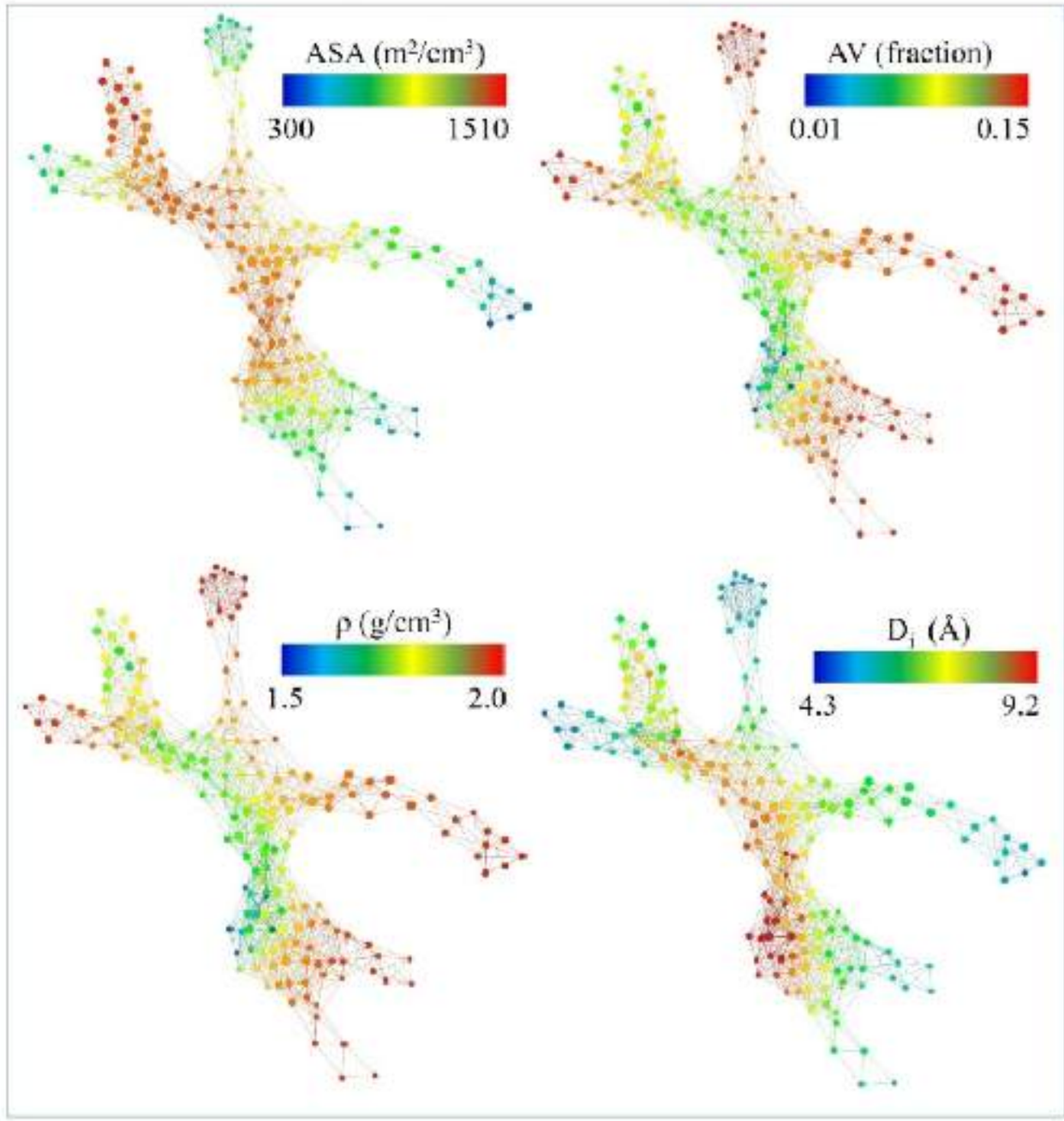
Diversity of Materials Databases

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

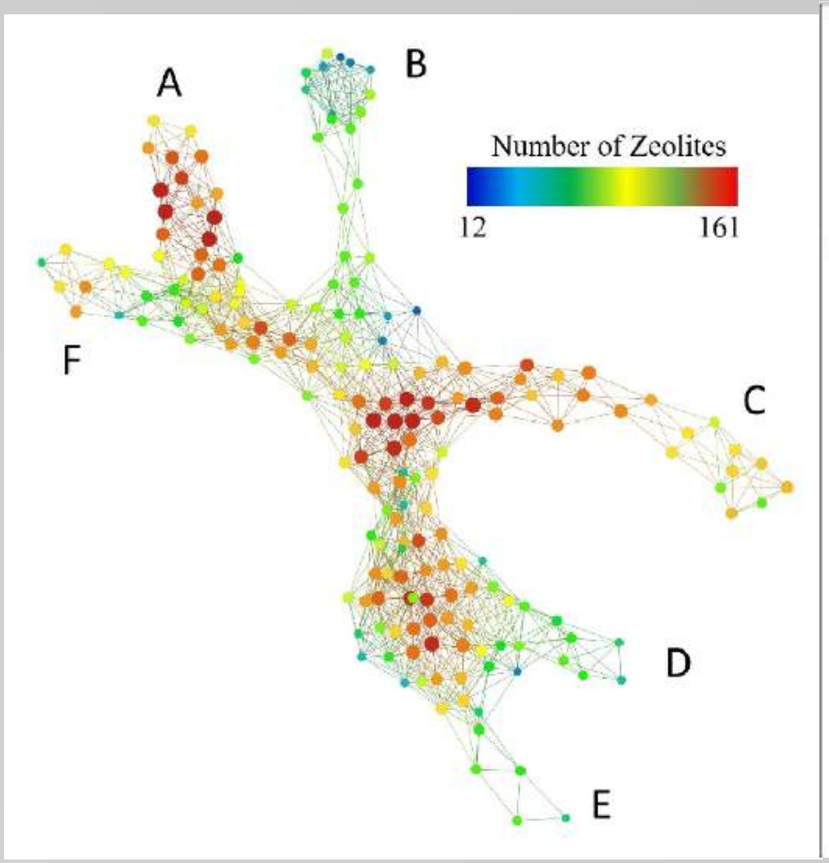


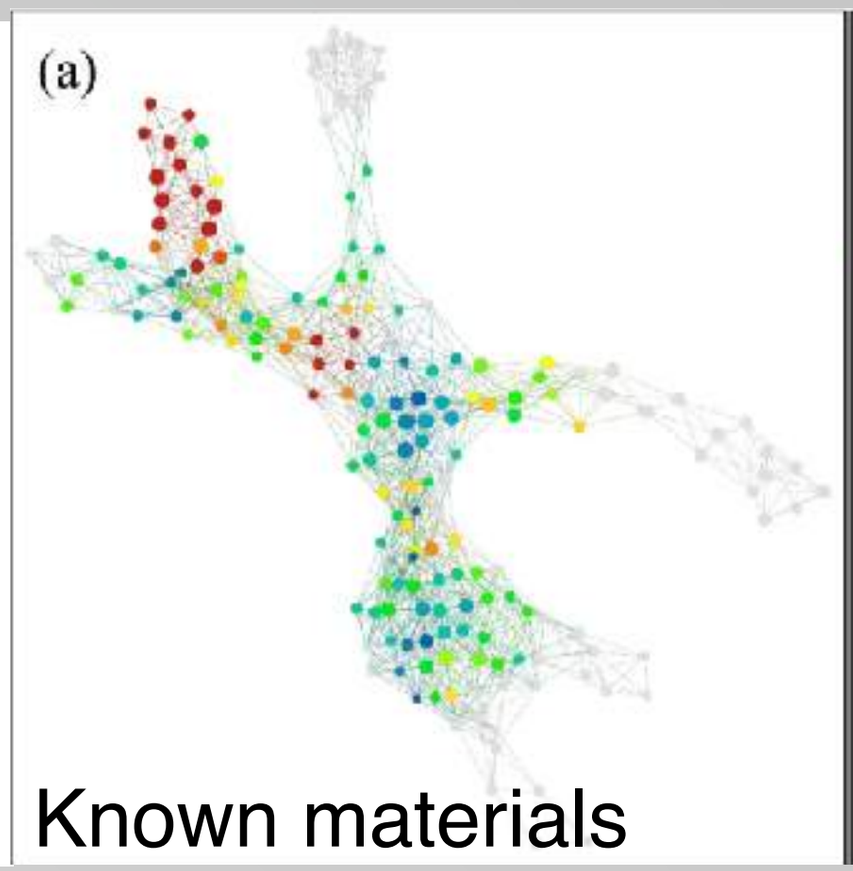
Diversity of zeolite structures



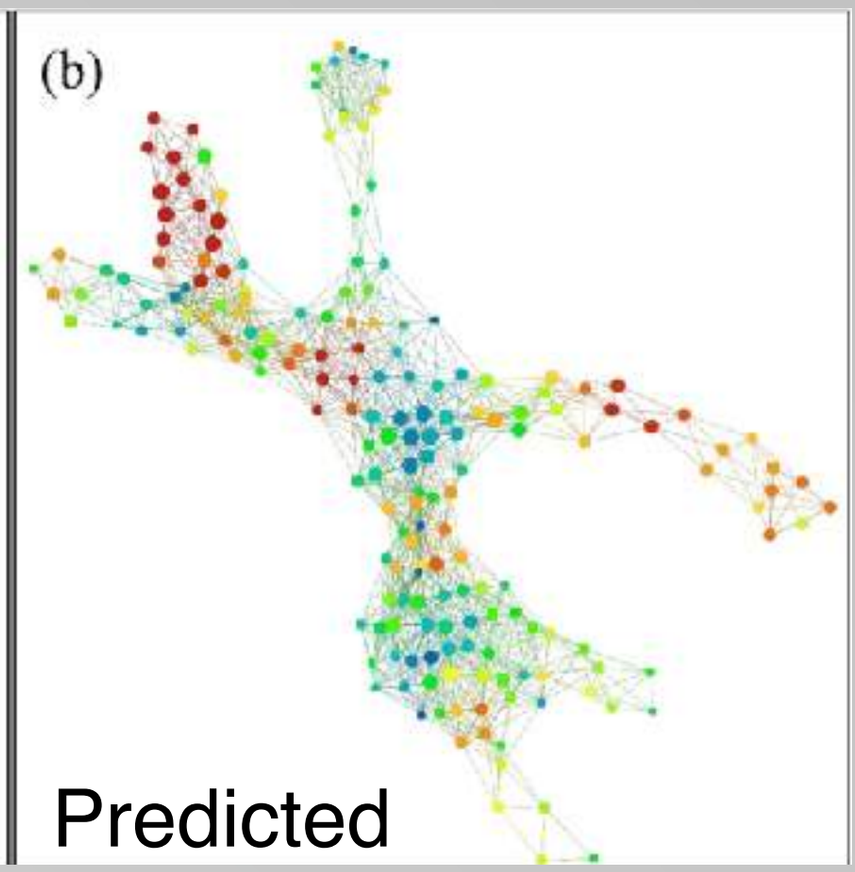


Diversity of zeolite structures

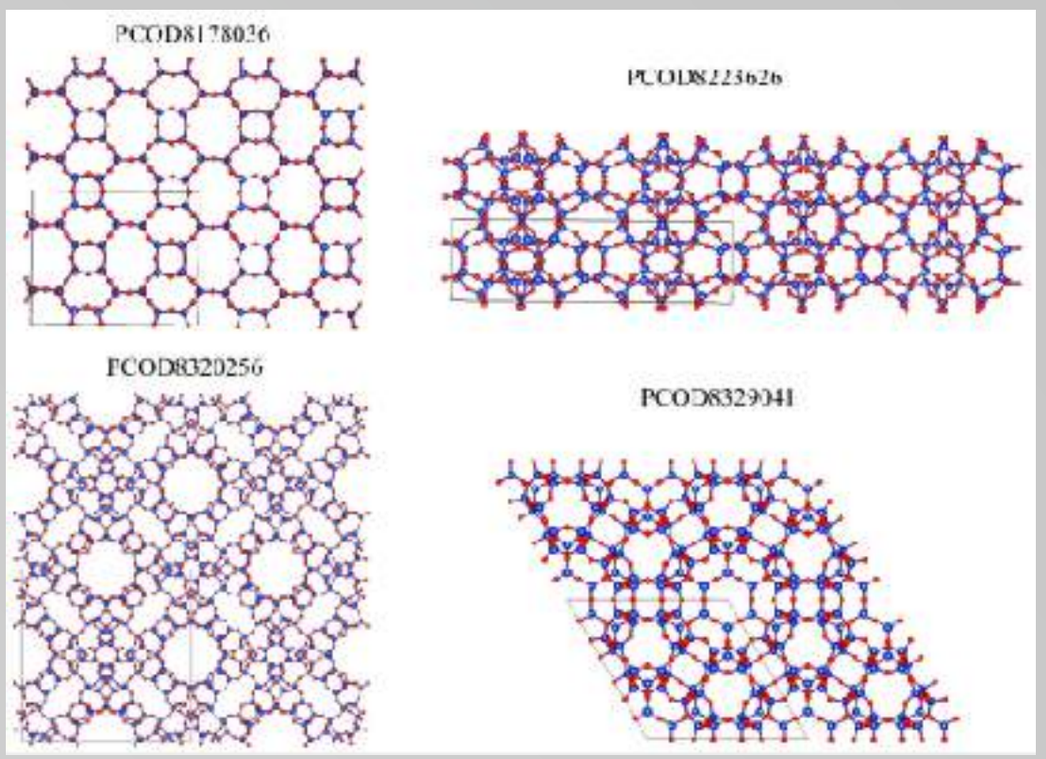




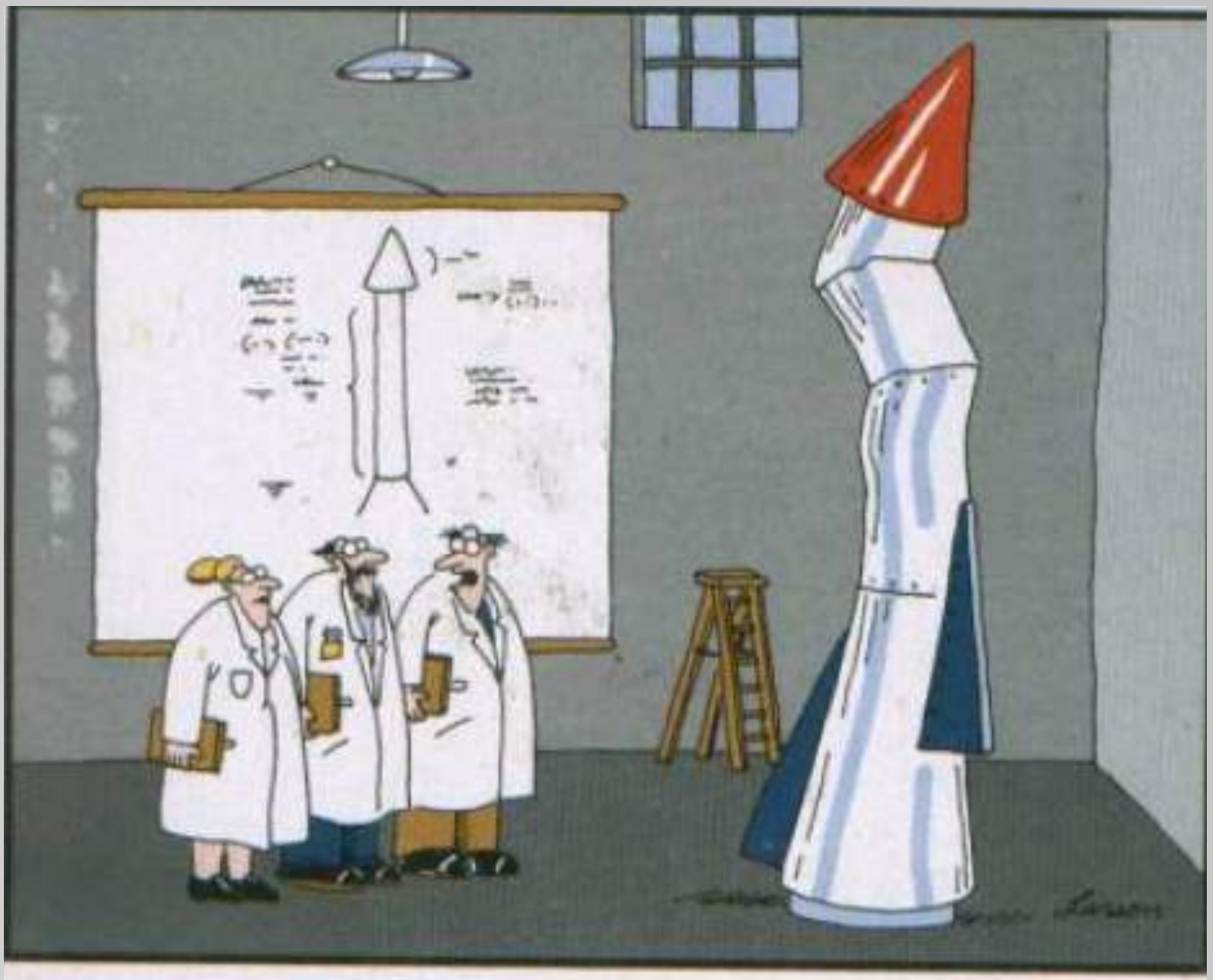
Known materials



Predicted

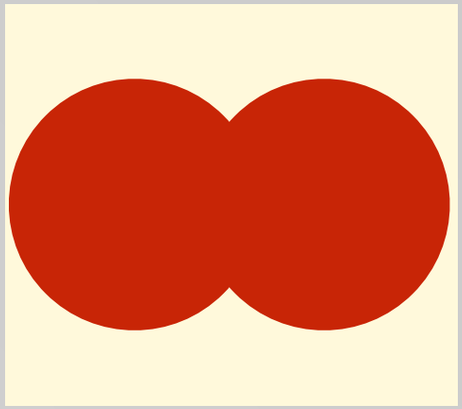


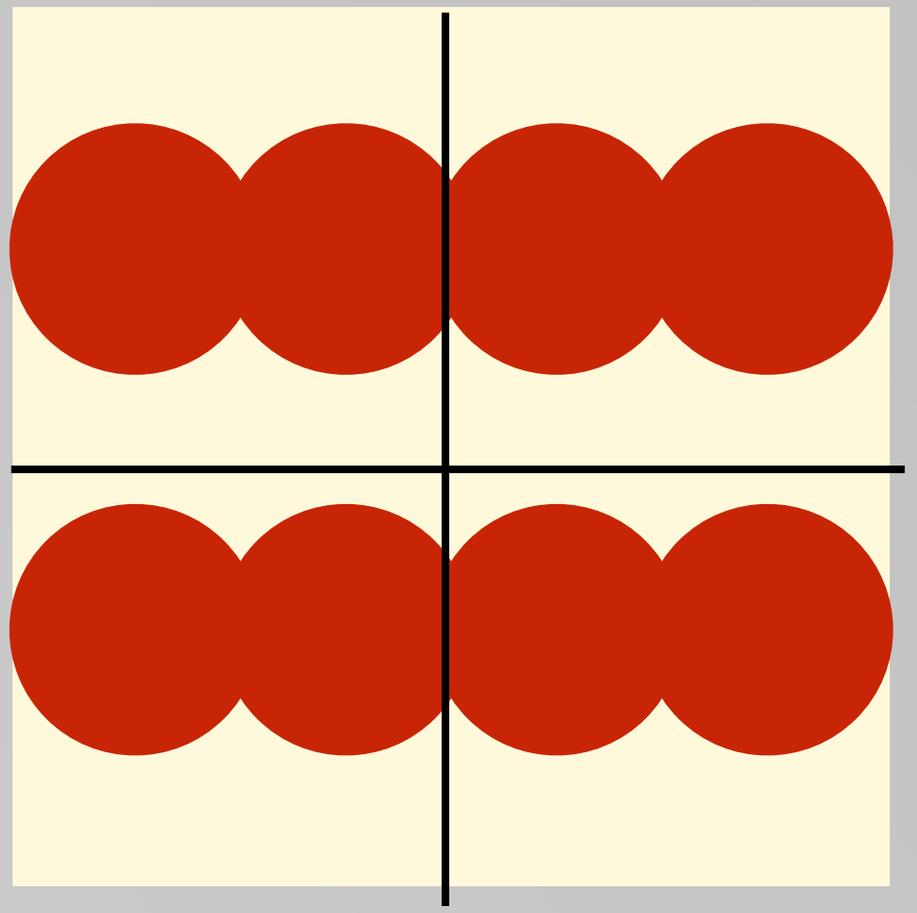
What does not work yet…

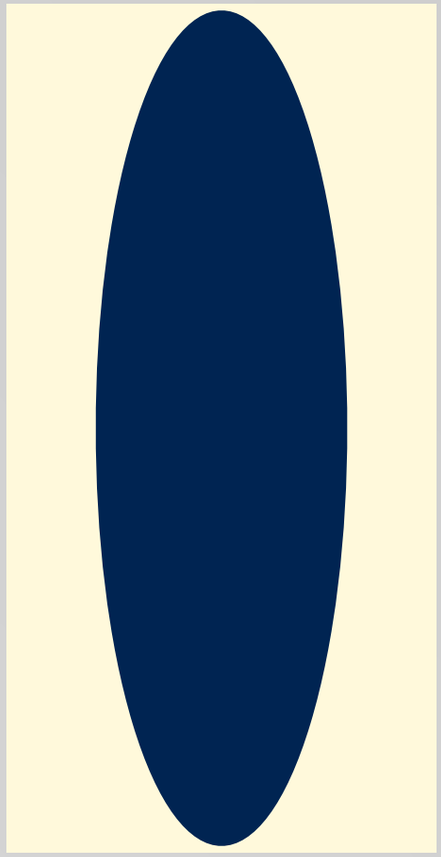


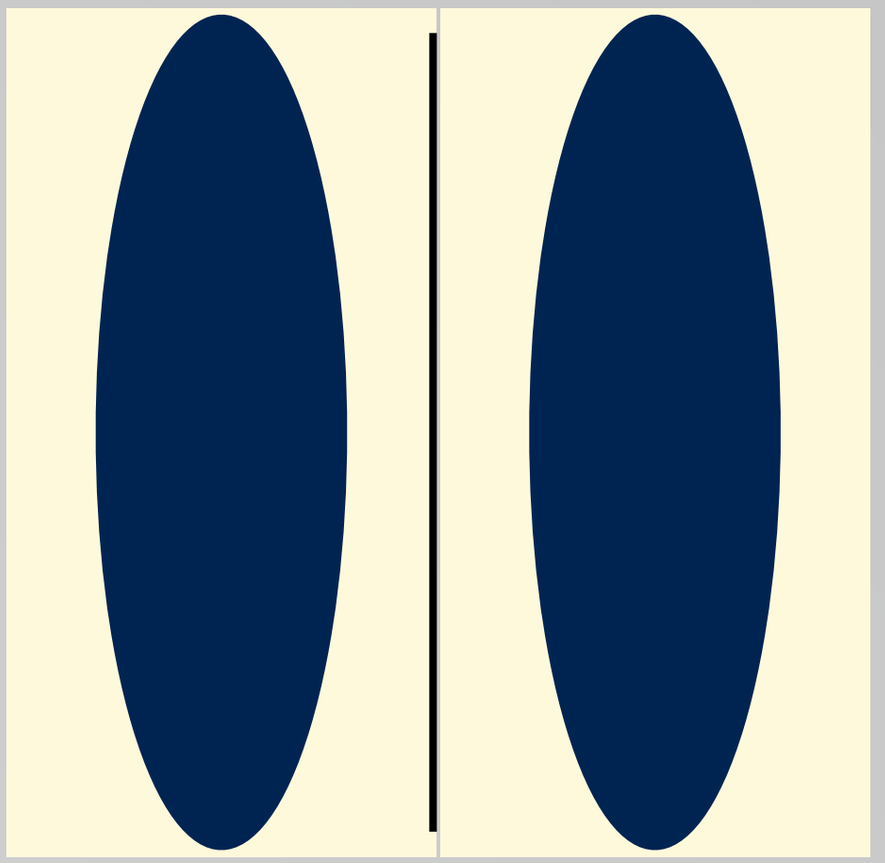
"It's time we face reality, my friends. …
We're not exactly rocket scientists."

Symmetry +
Periodic boundary conditions





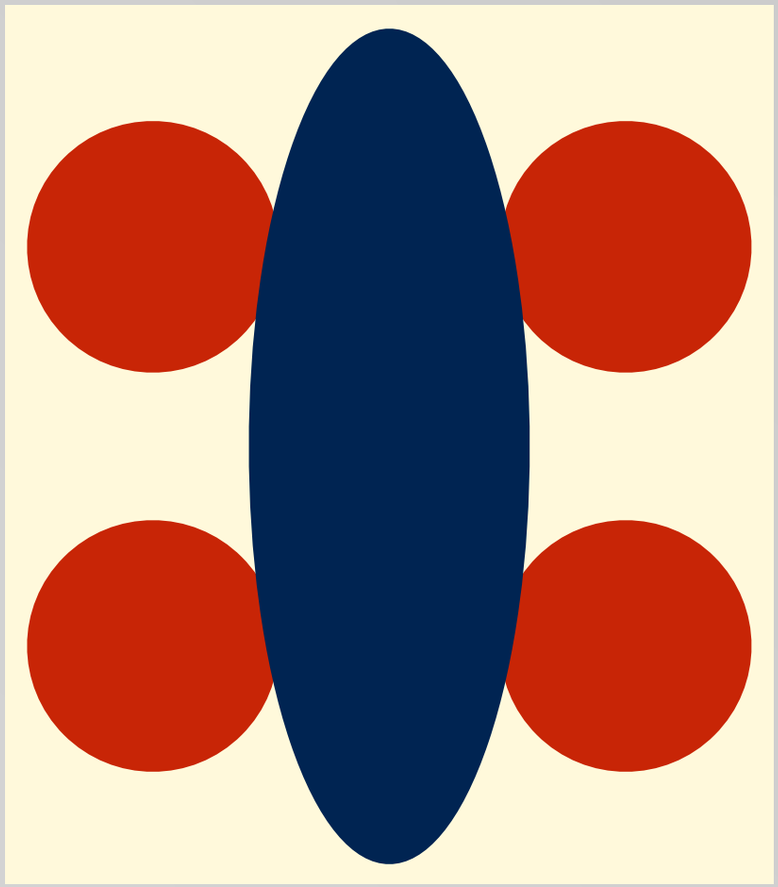


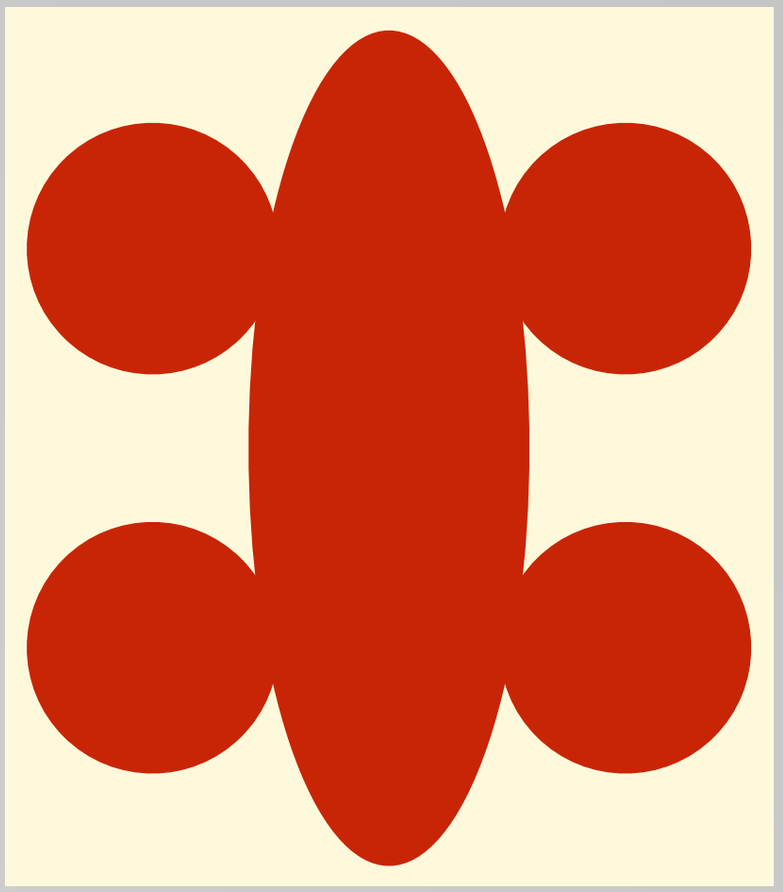


Probe

hydrogen

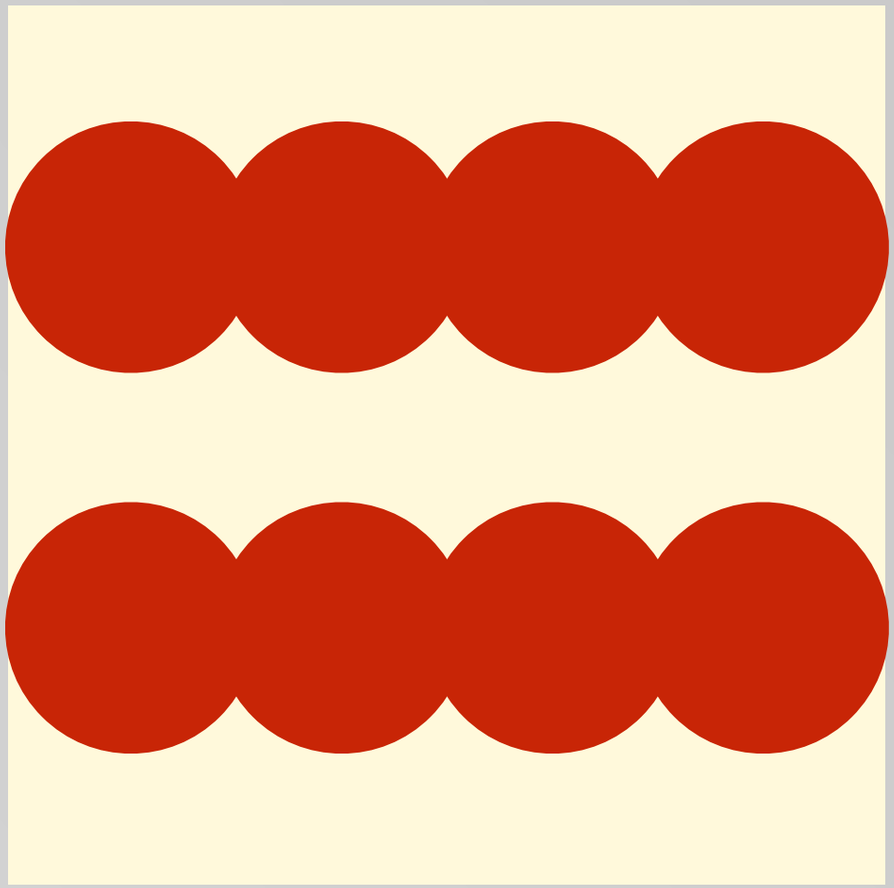
methane

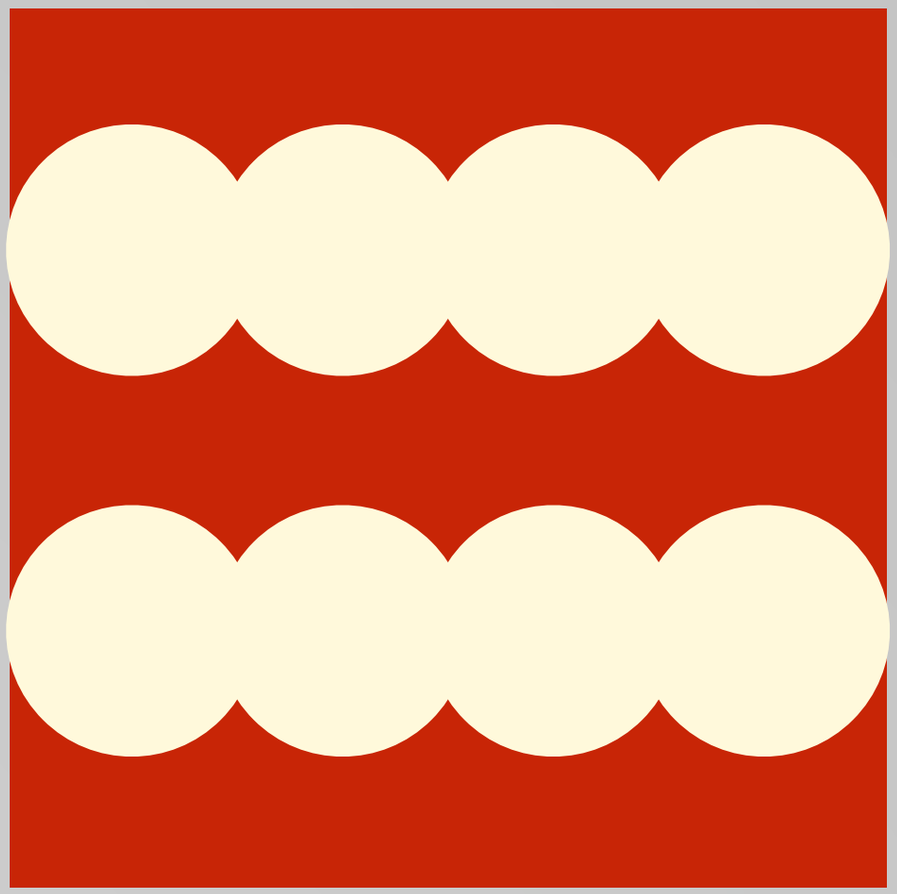




Solution: probe dependent fingerprint

Inside versus outside





Both have the same fingerprint, but not the same performance

Wish list

- **Too expensive**
  - we do not know how to take crystal symmetry into account
  - distance matrix too expensive to compute for 1’000’000 materials
- **Better description**
  - difference between the inside and the outside
- **No perfect understanding**
  - which distance to use for which property
  - Pore volume depends on the probe

Conclusions

- Methane storage
  - Best material: as many sites as possible with the right energy
  - ARPA-e targets are too optimistic
- Similarity
  - We have developed the language to express similarity
  - Nanoporous materials: we can now quantity the similarity of the pore structure
  - Similar pores similar performance
- Materials Genome:
  - Intelligence versus brute force ....
  - Screening for best materials: what can be obtained
  - Big-data science