Three examples of persistent homology applications in material science

Porquerolles meeting

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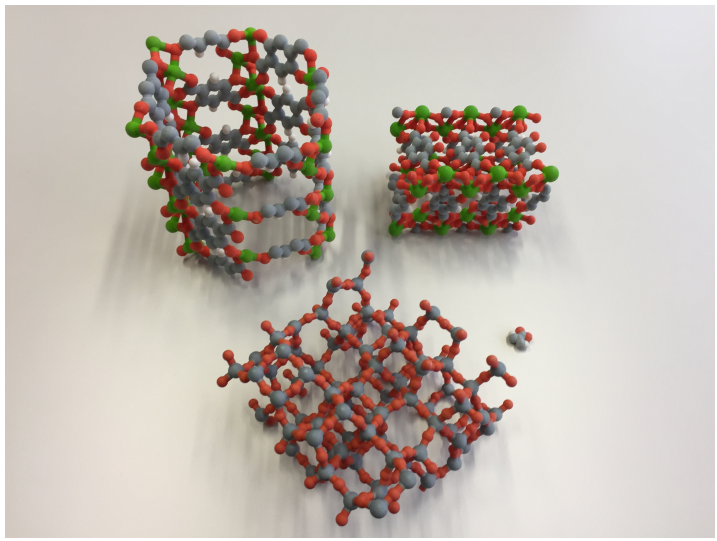


18 October, 2016

EPFL Valais

Energypolis ‘campus’ in Sion

Overview

Three applications:

- Description of pore shapes of nano-porous materials
- Analysis of hydrogen-bond networks in water
  (inside porous materials / model comparison)
- Prediction of ionic conductivity in super ionic conductors

Overview

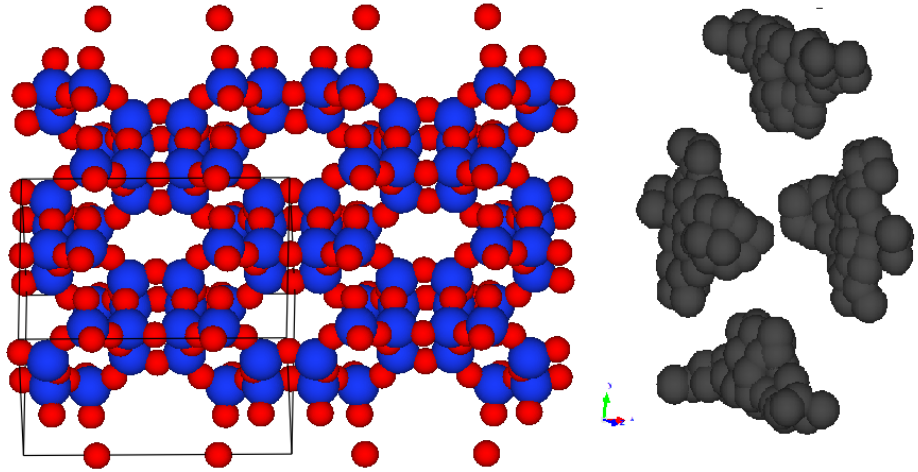
Three applications:

- Description of pore shapes of nano-porous materials
- Analysis of hydrogen-bond networks in water (inside porous materials / model comparison)
- Prediction of ionic conductivity in super ionic conductors

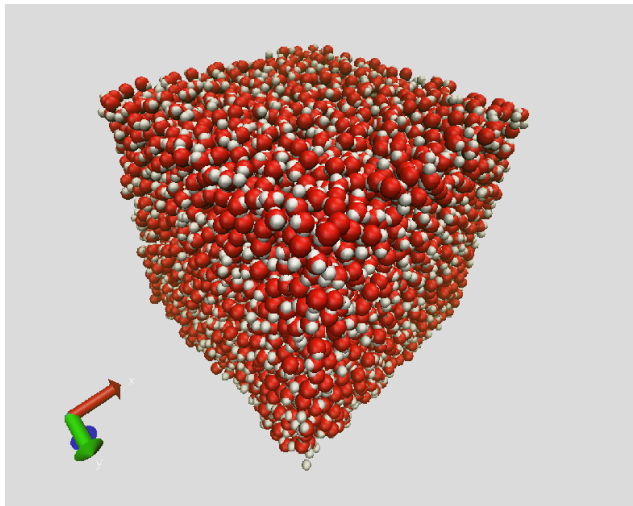
1. Typical settings
2. Describing pore shapes
3. Comparing water models
4. Water in metal organic frameworks
5. What is the right setting? Warning
6. Super ionic conductors
7. Typical questions

Let's dive straight in

i Structure described by points



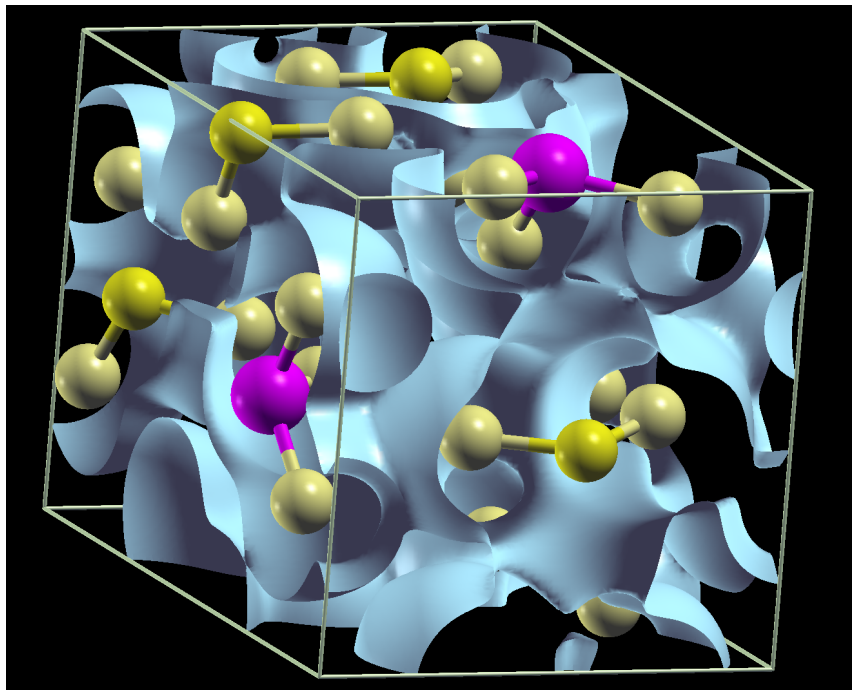
zeolite ITW



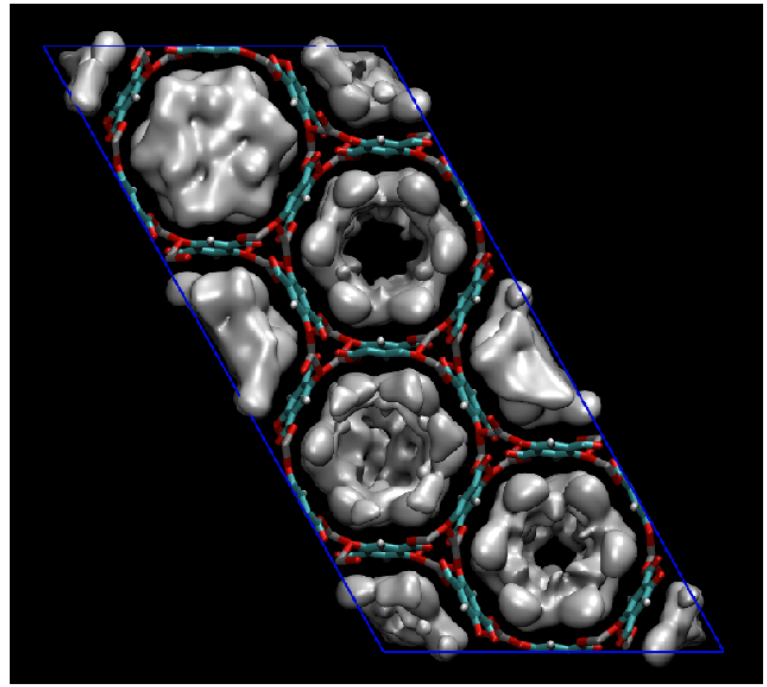
bulk water

Let's dive straight in

ii Structure described by a grid



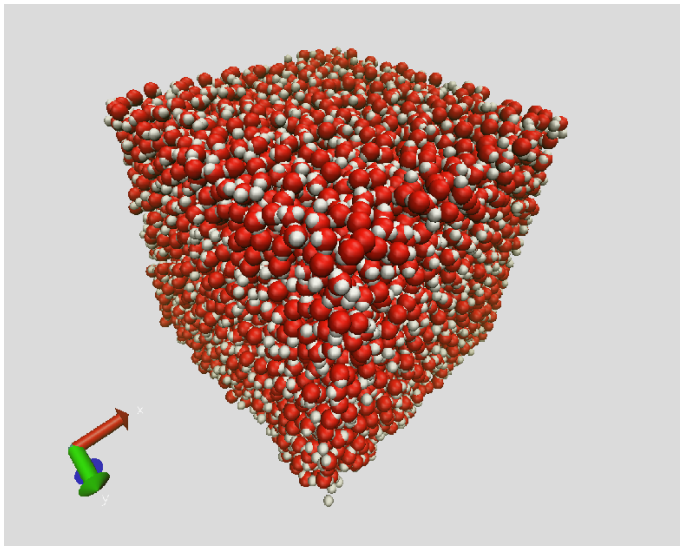
electron charge density

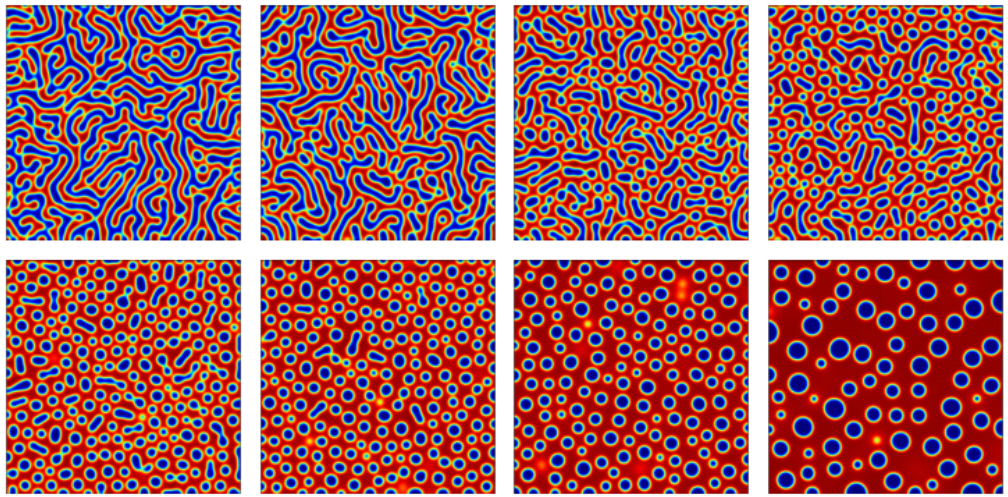


water probability

typical tasks

- screening $\leftarrow$ new descriptor for particular property (what is important to describe a property, which one?)
- averaging (from snapshots)



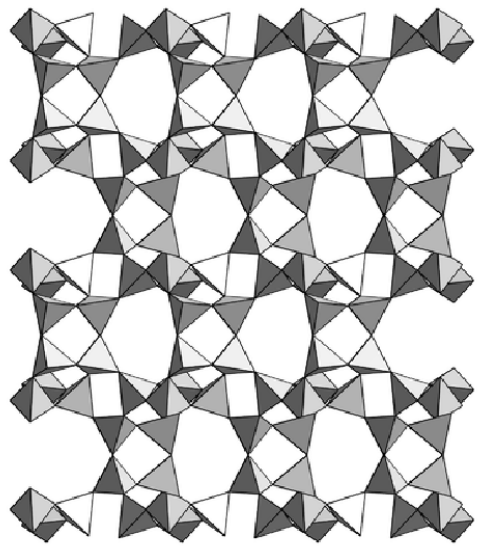


Paweł & Thomas' phase separation dynamics in binary metal alloys

Zeolites

Zeolites [$\zeta\epsilon\omega\ \lambda i\theta o\sigma$] boiling stone, up to 40 % water

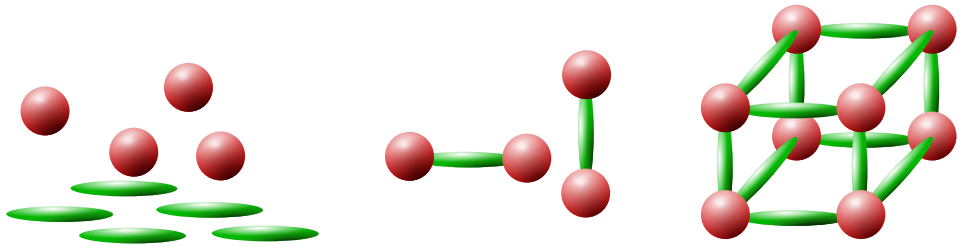
Nano-porous materials
Main industrial application:
Ion exchange in washing detergents to decrease water hardness.



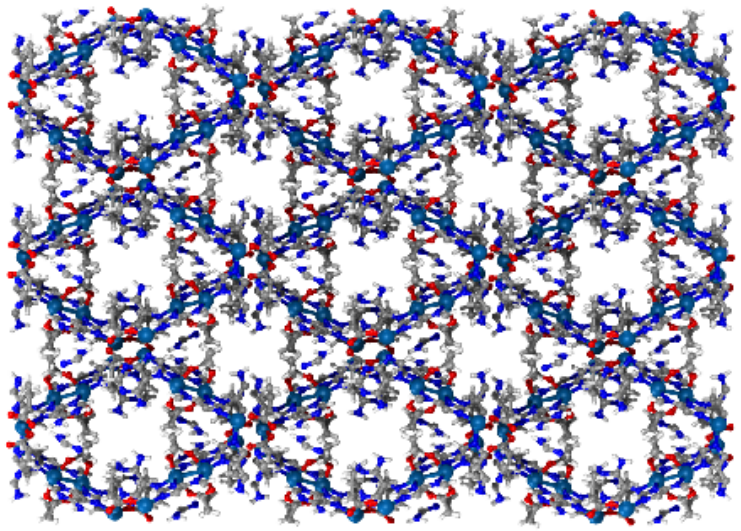
Zeolites consist of SiO_4-tetrahedrons

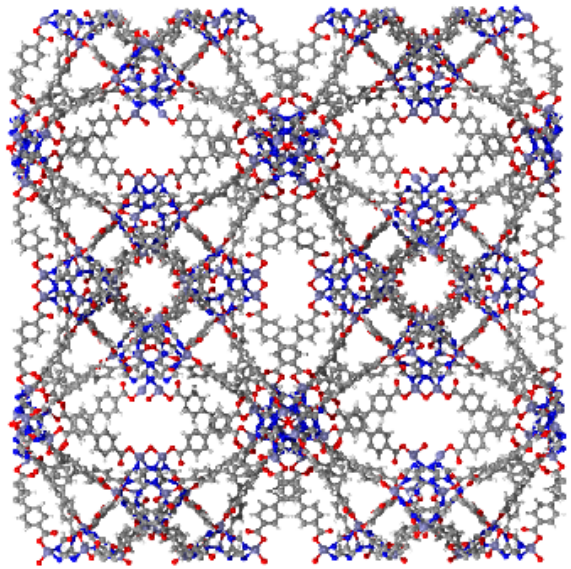
Metal organic frameworks (MOF's)

'Generalisation' of zeolites. Porous materials.



MOF's: organic linkers attached to metal centers





Pore geometries of nano-porous materials

Pore geometry of nano porous materials (zeolites, MOF's, etc) use persistent homology to

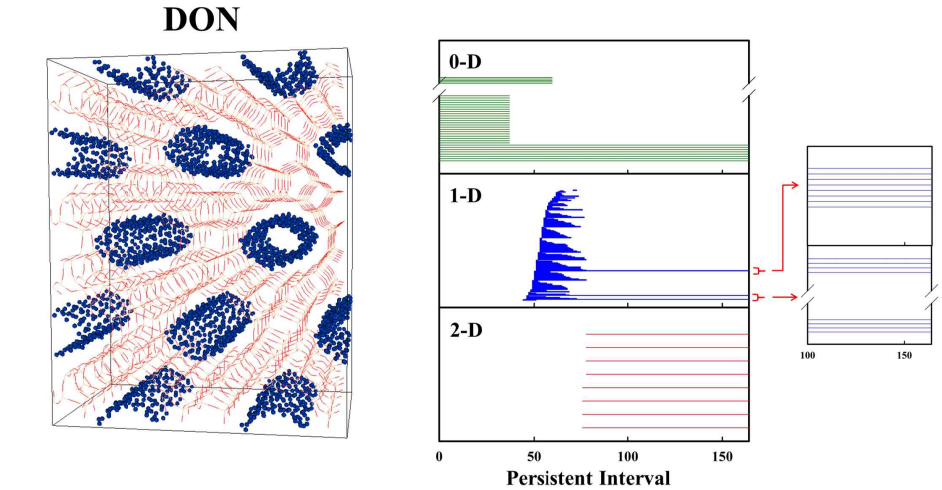
a develop a descriptor capturing the geometry of pores
   $\rightarrow$ quantify similarity,
   $\rightarrow$ compare,
   $\rightarrow$ classify materials by shapes

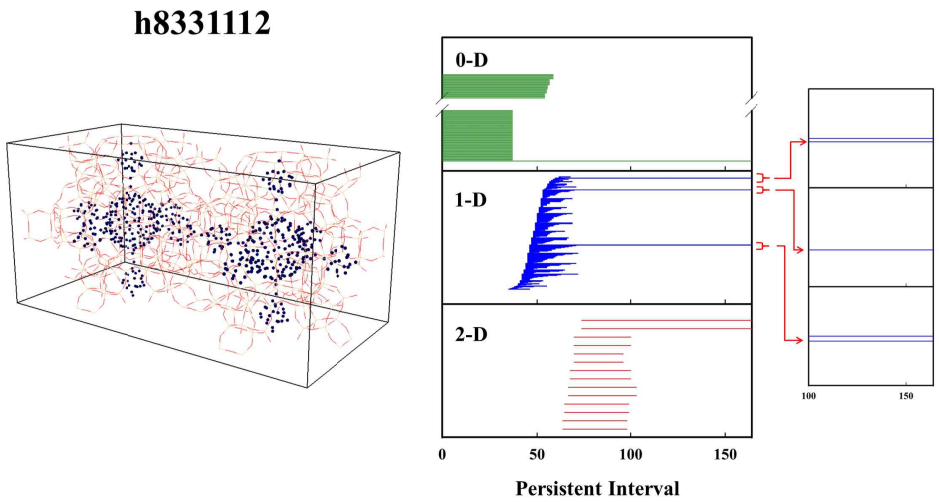
b illuminate the topography of material libraries
   $\rightarrow$ distinct classes of top-performing materials,
   $\rightarrow$ different optimisation strategies

Pore geometries of nano-porous materials

1.a) Development of a pore shape descriptor:

1. Sample the pore surface
2. Construct the Vietoris-Rips complex
3. Compute the 0-, 1-, 2-dimensional homologies



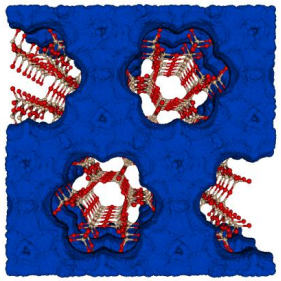
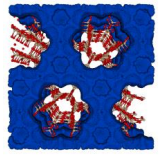
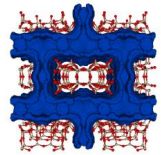
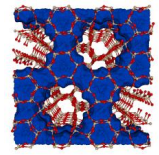
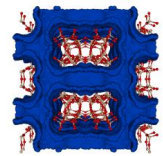
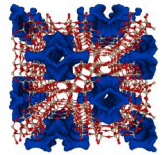
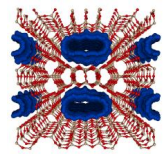
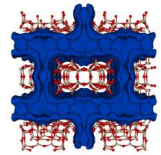
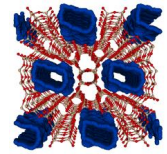
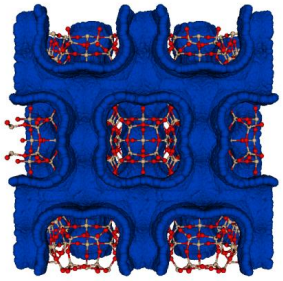
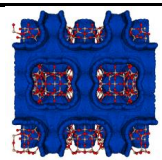
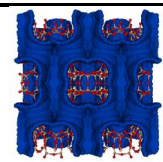
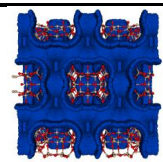
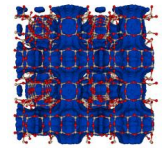
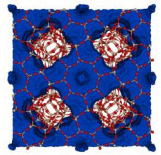
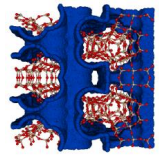
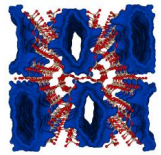
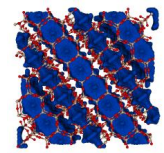


Pore geometries of nano-porous materials

1.a) Development of a pore shape descriptor

$\rightarrow$ quantify similarity,

$\rightarrow$ search for similar structures

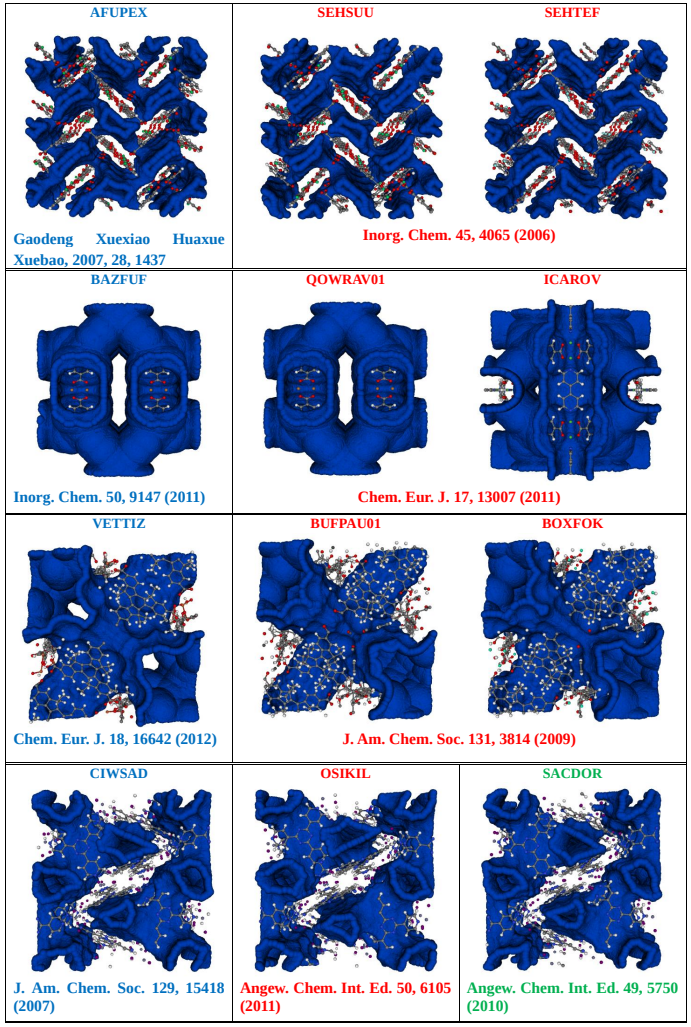
Seed	Descriptor	Selected Nth Similar Structure 1st	2nd	3rd	4th
SSF 	PerH				
	ConD				
IWV 	PerH				
	ConD				

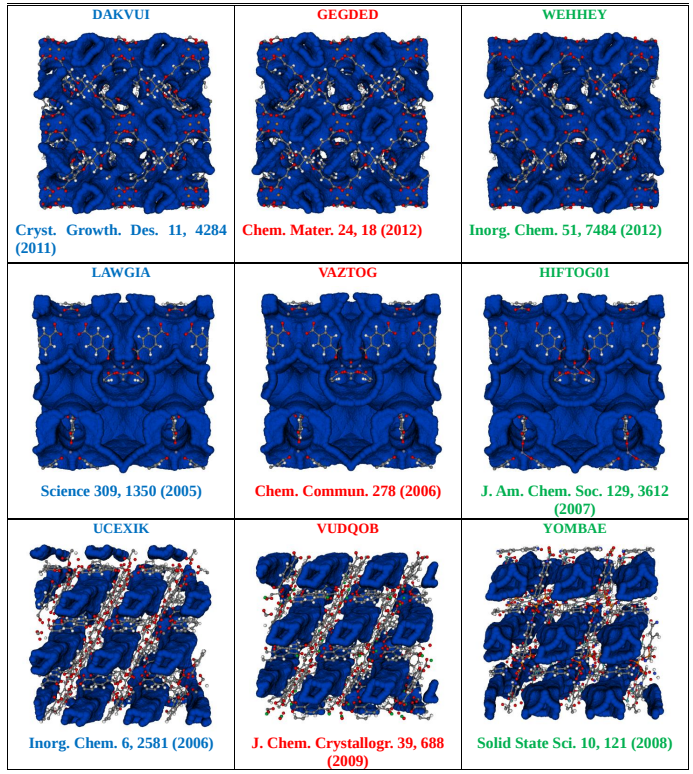
Pore geometries of nano-porous materials

1.a) Development of a pore shape descriptor

$\rightarrow$ quantify similarity,

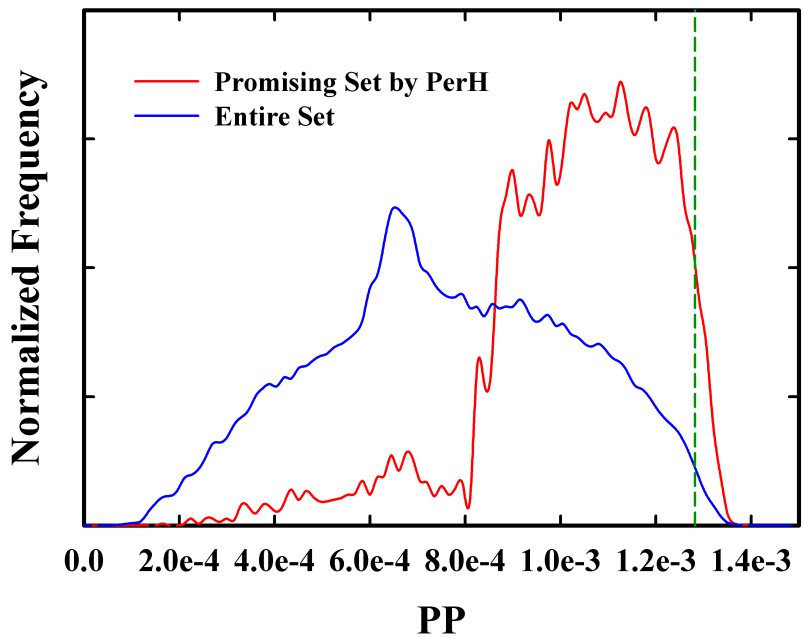
$\rightarrow$ search for similar structures

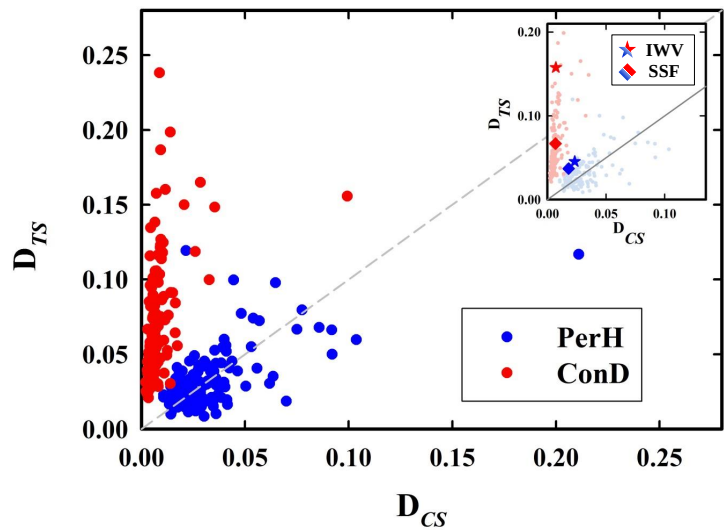




Pore shape matters!

- Pore shape is related to performance (carbon capture, methane storage, etc)
- and doing better than conventional descriptors

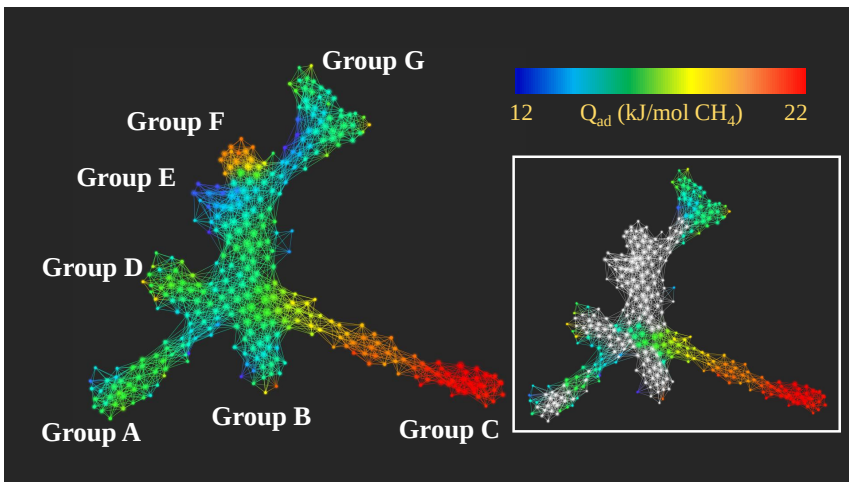


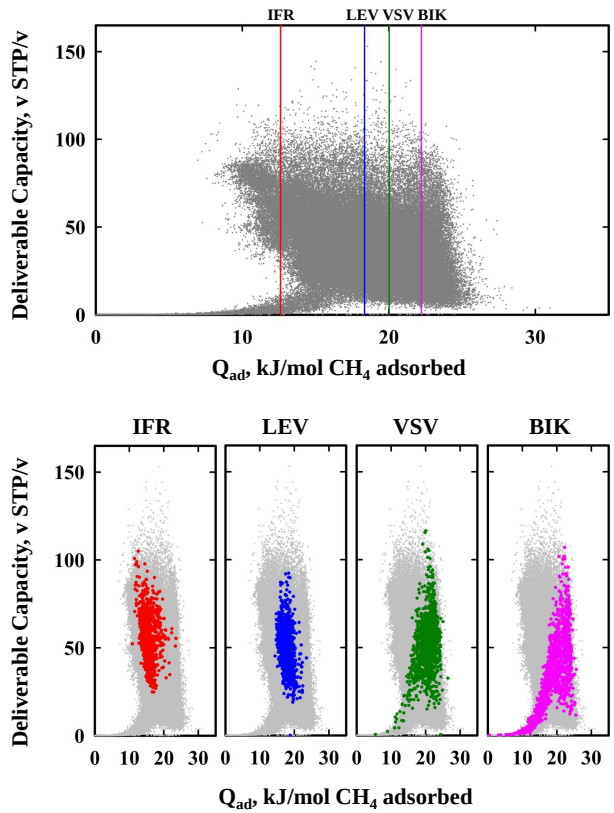


Pore geometries of nano-porous materials

1.b) Topography of zeolites

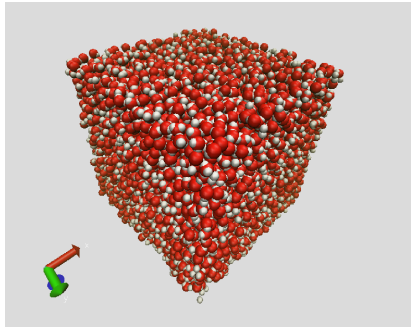
- Diversity of top-performing structures
- 6 different classes of pore-shapes
- Optimise within a class, e.g., heat of adsorption



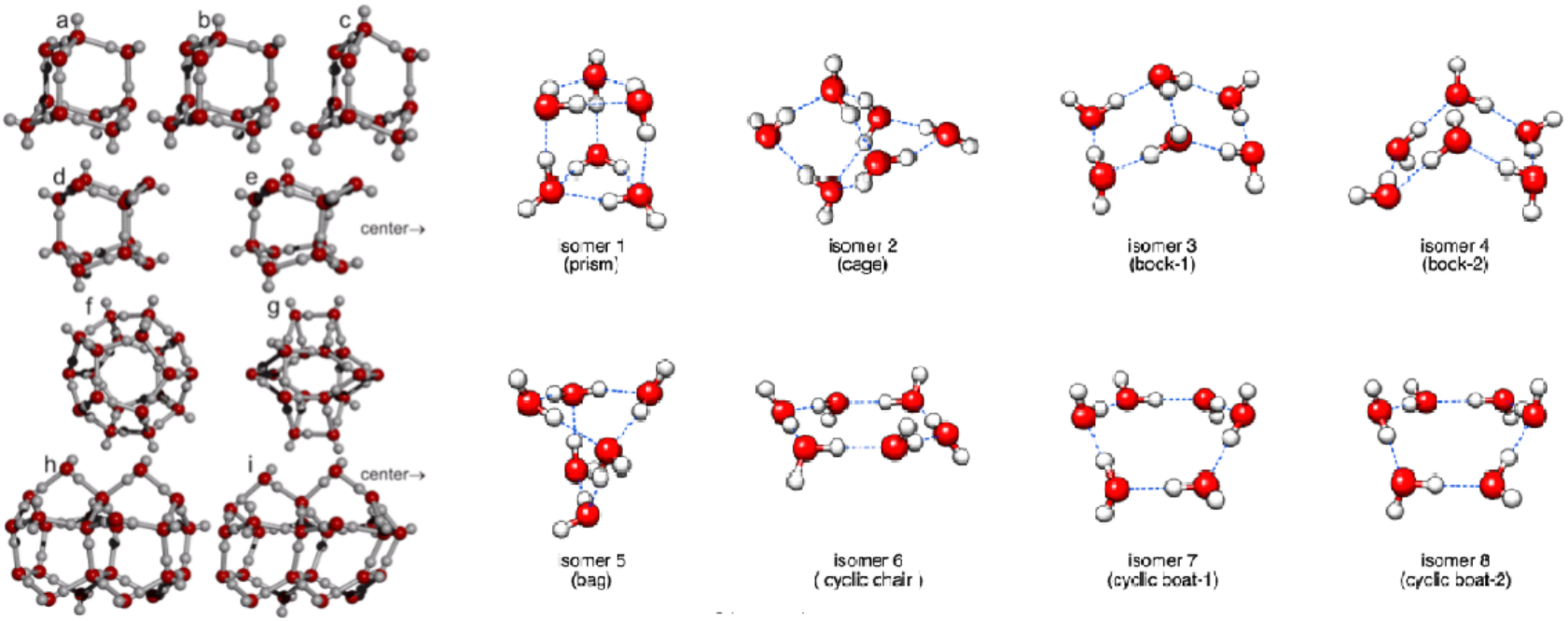


Hydrogen bond networks in H_2O

- Comparing different models
- Get correction terms
- Experimentally known is only averaged atom number around each atom per distance (RDF)



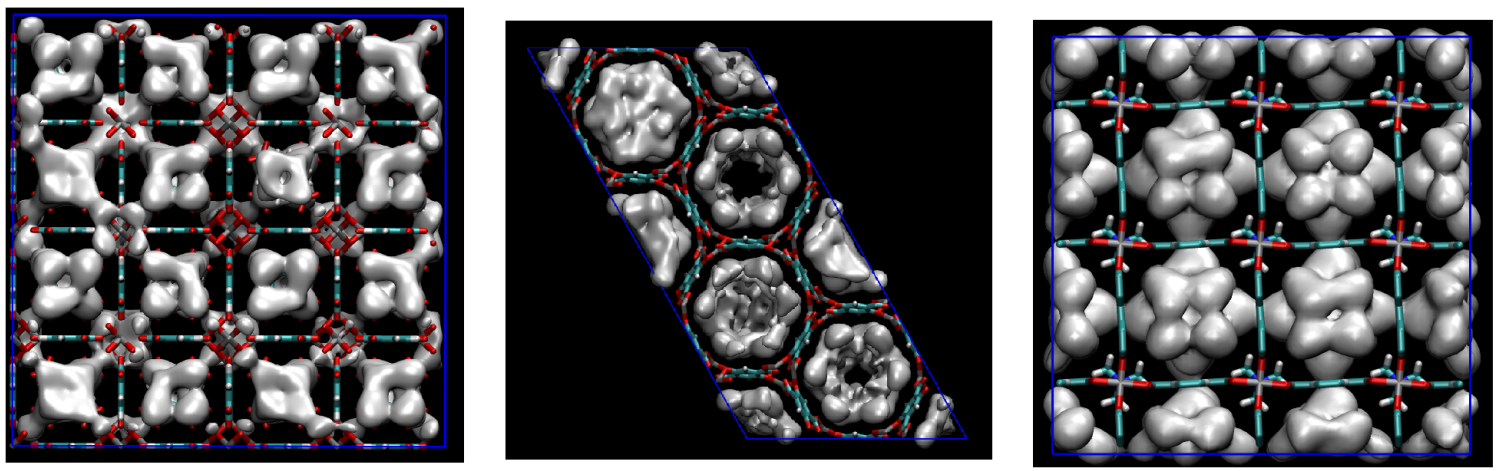
bulk water



Formations in H bond networks

Hydrogen bond networks in H_2O

- Water inside MOF's
- Perform simulations of bulk water and water in MOFs.
  Ranking a MOF based on how little it 'disrupt' the PH of bulk water.
- What hydrogen bond network forms?
  How dependent of the shape of the pores?



Water density inside MOFs

⚠ WARNING ⚠

- 'What do you want?' answered by 'What can you do?'
- users take ph-output as intrinsic property/as fixed tool Interpretation?
- will give you anything (unmotivated) to get insight, demanding unsupervised analysis to find the unknown. Instead: know your system

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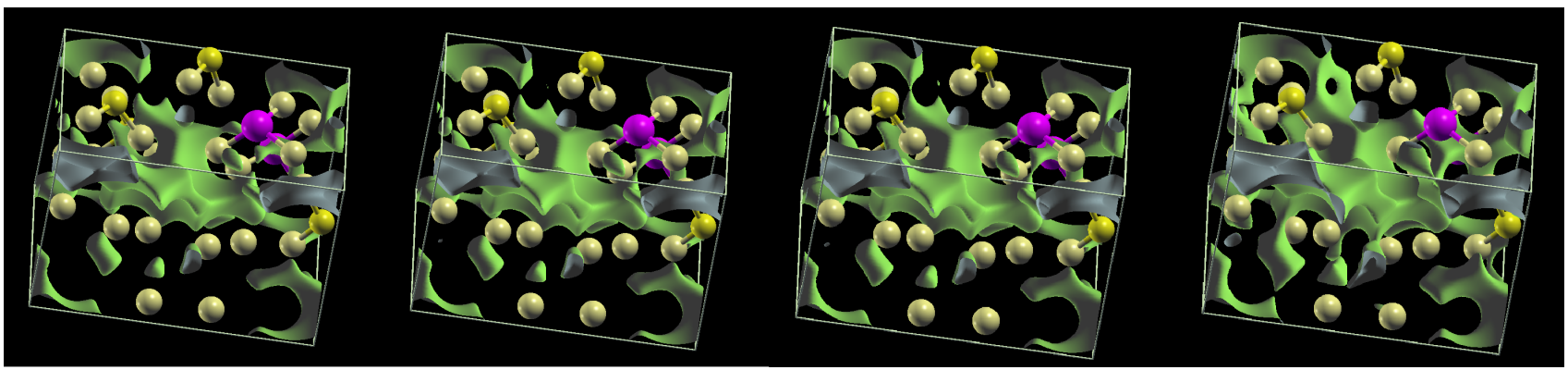
1. worst case: User works blindly with software
2. second worst case: We are performing the analysis unsupervised for them, underestimating the complexity and uniqueness of each application
3. further problem: slow thinking mathematician
4. desired: Know what you are looking for and modify your analysis accordingly instead of using (random) results as guidance. Problem: Impatience, try and error approach, constructive instead of specific approach

Conductivity of super ionic conductors

Predicting and screening for ionic conductivity of Li conductors

- When do channels close – diffusion & temperature
  $\rightarrow$ death time of 1-dimensional homology classes to predict activation energy of diffusion
- 'dimensionality' of diffusion
- sizes of channel system
- minimal value along a paths, all values along a path (same info back as scalar function)



Electron charge density iso-surfaces

Conductivity of super ionic conductors

(loading video)

Typical questions

- using symmetries
- periodicity (non-orthogonal)
- weighted Voronoi decompositions
- path detection, dimensionality, independence
- properties along paths (barriers, diameters, min value, long parts of tunnels with particular size, adsorption sites . . .)
- connected component detection

Thank you!

for your attention

Thanks to the people on the projects

LSMO	Yongjin Lee
	Seyed Mohamad Moosavi
	Amber Mace
	Matthew Witman
	Berend Smit
THEOS	Leonid Kahle
	Aris Marcolongo
INRIA	Paweł Dłotko
UPHESS	Kathryn Hess

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