Using persistent homology to characterise MOFs

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9 June 2017

The story so far...

Idea

- How do we characterise pore geometry at different length scales?
- For each MOF, compute a barcode using **persistent homology**!

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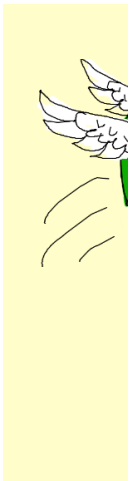

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ARTICLE

Received 24 Feb 2017 | Accepted 27 Mar 2017 | Published 23 May 2017

DOI: 10.1038/ncomms15396 OPEN

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In most applications of nanoporous materials the pore structure is as important as the chemical composition as a determinant of performance. For example, one can alter performance in applications like carbon capture or methane storage by orders of magnitude by only modifying the pore structure. For these applications it is therefore important to identify the optimal pore geometry and use this information to find similar materials. However, the mathematical language and tools to identify materials with similar pore structures, but different composition, has been lacking. We develop a pore recognition

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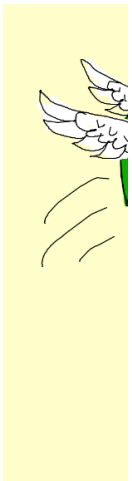

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How will our approach differ?

In the paper

Barcode based on MOF + size of sorbate molecule	One similarity measure	Was able to link barcodes similarities to MOF performance (methane storage)

Our approach

Barcode based on MOF	Similarity measure that depends on sorbate molecule	Can we link barcode similarities to MOF performance?

How will our approach differ?

In the paper (expensive) (particular) (works!)

Barcode based on MOF + size of sorbate molecule	One MOF similarity measure	Was able to link barcodes similarities to MOF performance (methane storage)

Our approach (cheaper) (general) (works?)

Barcode based on MOF	MOF similarity measure that depends on sorbate molecule	Can we link barcode similarities to MOF performance?

How will we achieve this?

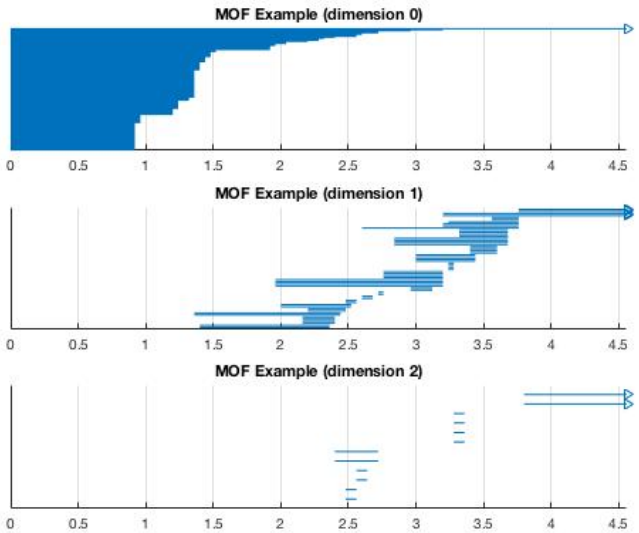
Step 1: Compute barcodes

MOF atoms

x, y, z

coordinates

JavaPlex



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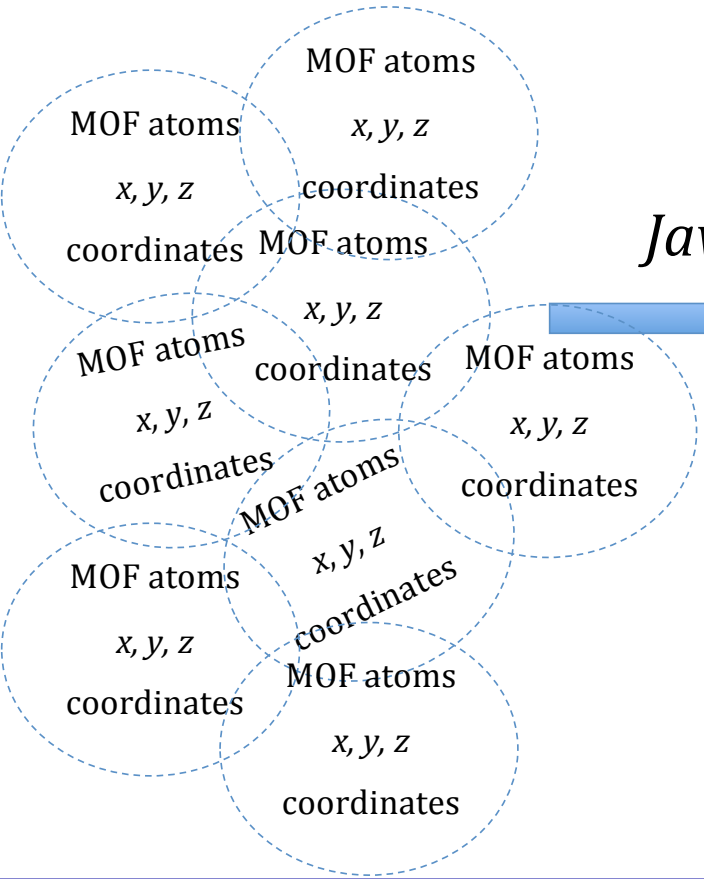

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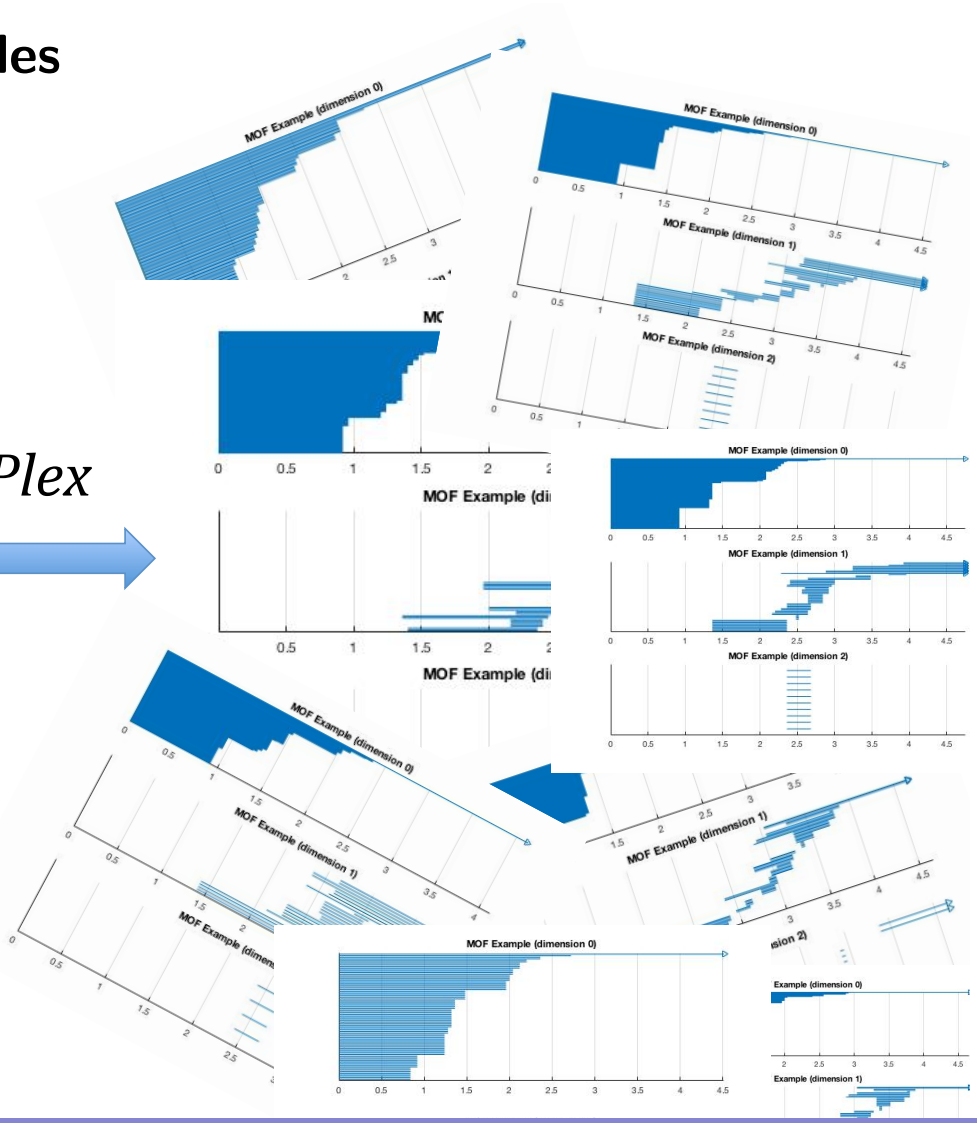

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Step 2: Define MOF similarity measure

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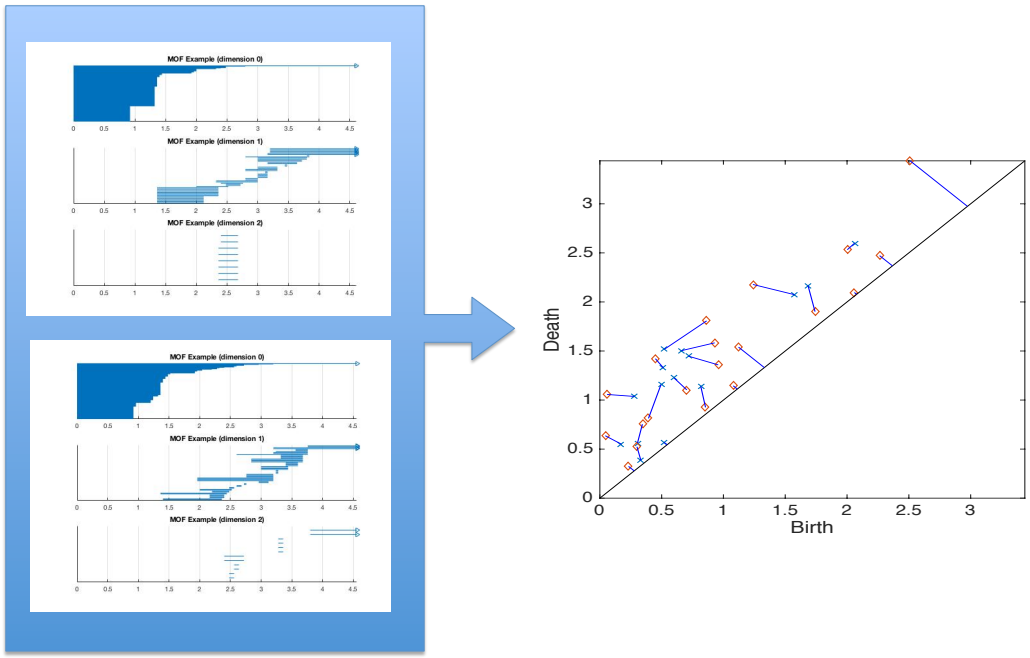
Persistence diagrams



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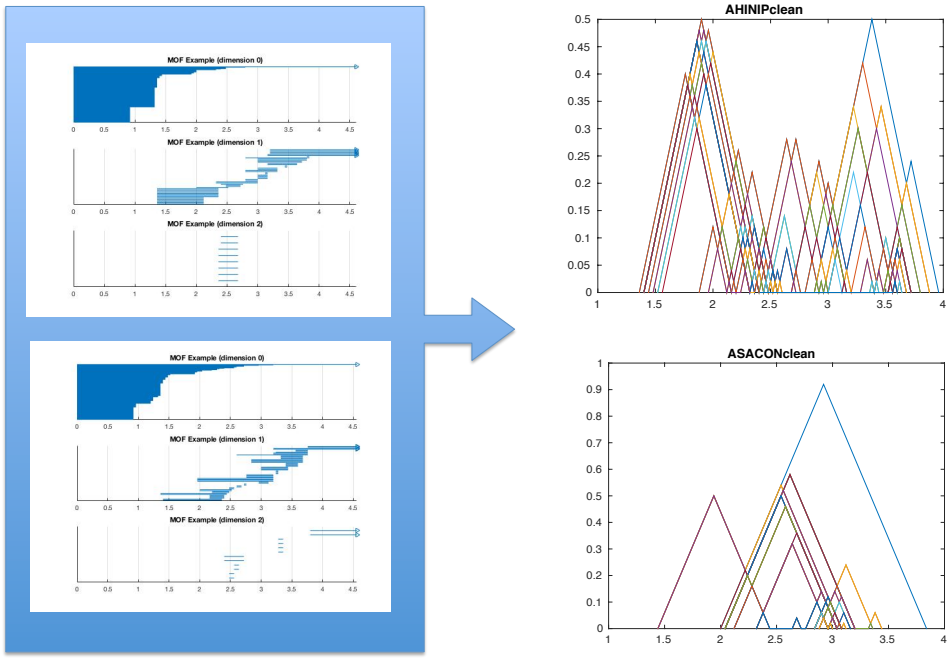
Persistence landscapes



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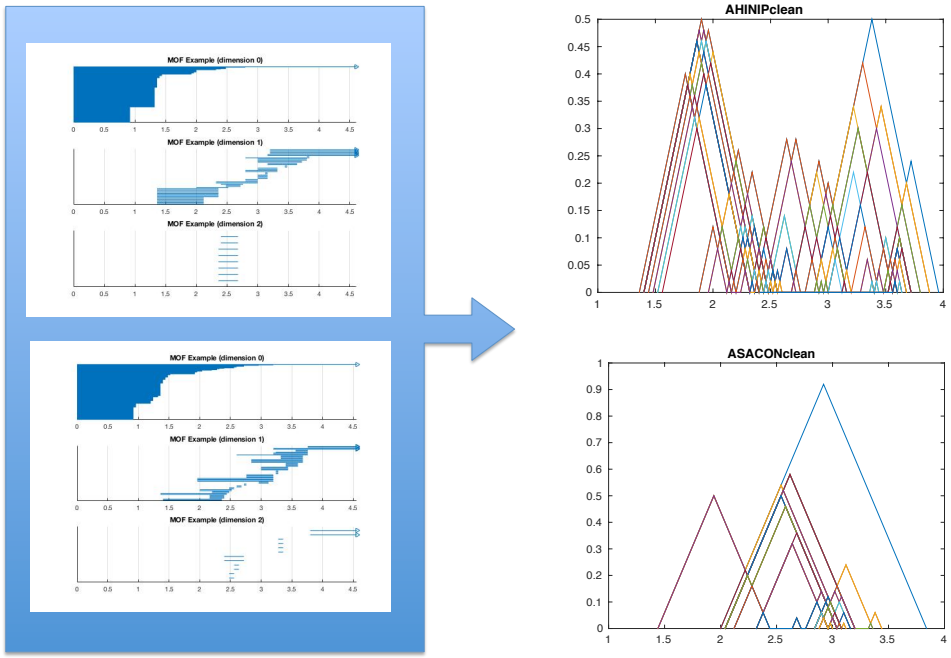

Different similarity measures for different sorbates - e.g. higher weights on scales similar to sorbate size

How will we achieve this?

Step 3: Choose the best distance measure

- **Aim**: Find similarity measure that gives best predictions of MOF performance
- **Method**: Gaussian process regression (Kriging)

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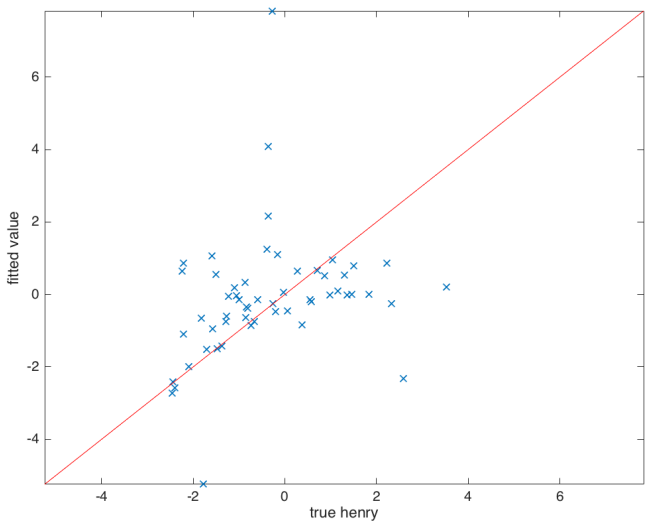
Is there a correlation between MOF similarity and MOF performance?



- MOF similarity: Using persistence diagrams
- MOF performance: Water molecule adsorption (Henry)

Future work

- Experiment with diff erent MOF similarity measures, in particular, from persistence landscapes
- Use bigger data set
  - more MOFs
  - different sorbates

- MOF categorisation tailored to sorbates
- Optimal MOF design for given application
- Optimal simulation sampling