Using persistent homology to characterise MOFs

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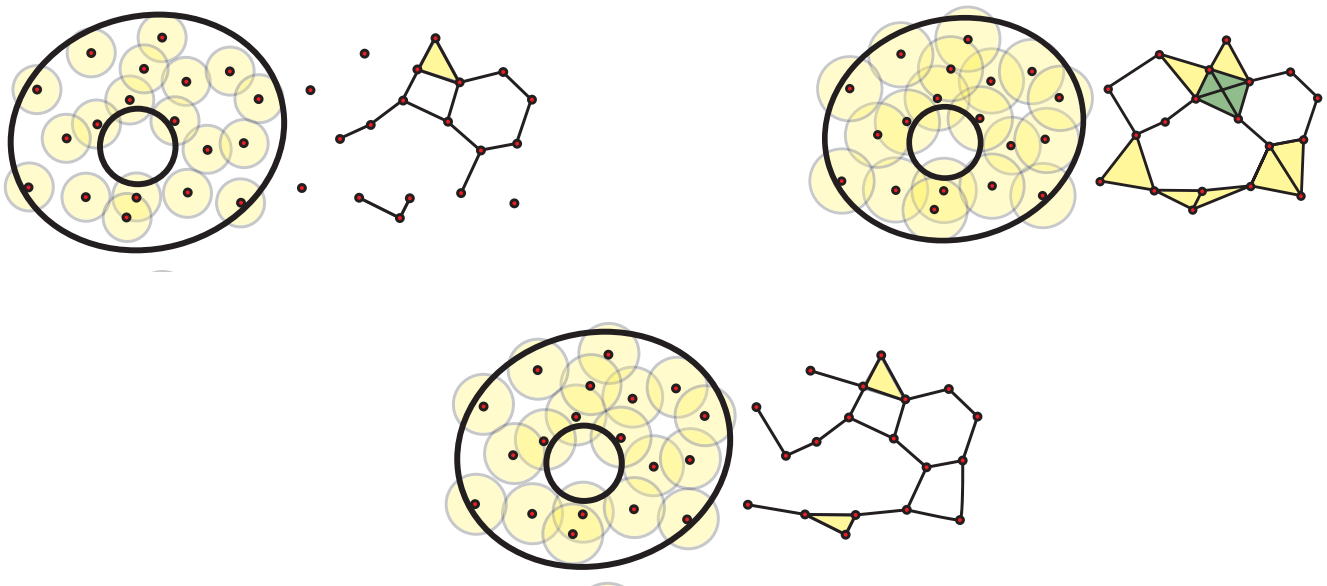
Idea

- How do we characterise pore geometry at different length scales?

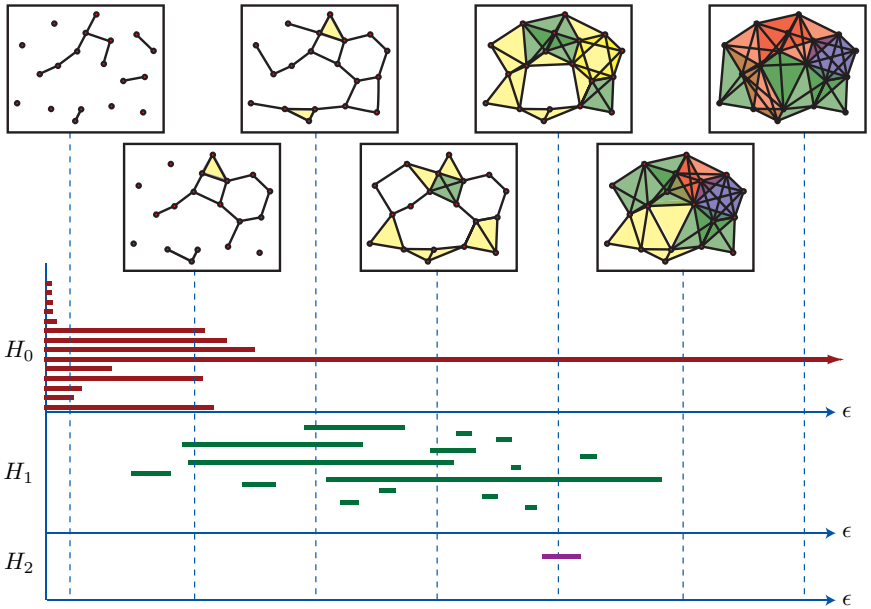
- Compute barcodes using **persistent homology**!
- **Hypothesis**: MOFs with similar barcodes will have similar behaviour.

What is persistent homology?

- Consider the atoms in the MOF as points
- For each $r > 0$, build a simplicial complex



What is persistent homology?



- Barcode encodes information on
  - the number of holes through which molecules can pass
  - at what length scale they exist

What do we plan to do?

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Quantifying similarity of pore-geometry in nanoporous materials

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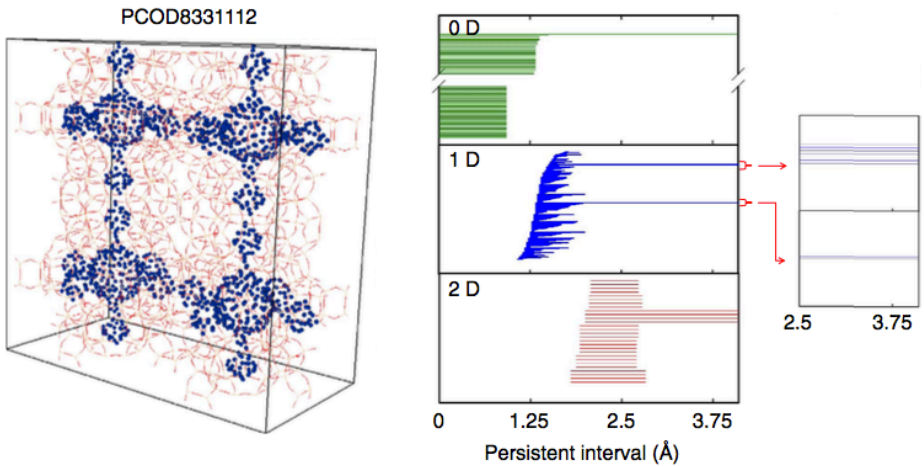
In most applications of nanoporous materials the chemical composition as a determinant of perfo performance in applications like carbon capture or r by only modifying the pore structure. For these to identify the optimal pore geometry and use thi However, the mathematical language and tools t structures, but different composition, has been la



What do we plan to do?

- Refine approach: use varying atom sizes
- Explore other options for measuring similarities and check for robustness with respect to noise
- Use barcodes for classification
- Take into account different applications (not just methane storage)
- Create a MOF-molecule performance matrix based
  - Compressed matrix based on classification
  - Use optimised sampling based on correlation structure of MOFs