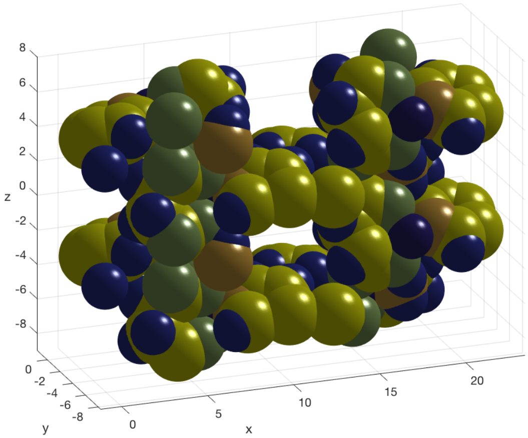
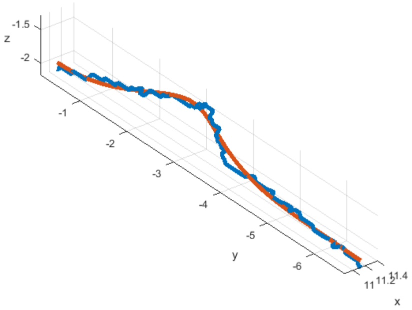
Using Differential Geometry to Classify the Shape of Pores in Metal-Organic Frameworks

Here is a MOF: show video



Smoothing out the curve by FFT



- Let $\gamma : [0, L) \to \mathbb{R}^3$ describe the noisy path.
- Regularise the path using $\gamma_{reg}(t) = (\gamma * g)(t)$ where $g(t)$ is the top hat function $\chi_{[-\epsilon,\epsilon]}$.
- Take the Fourier transform: $\hat{\gamma}_{reg}(\omega) = \hat{\gamma}(\omega)\hat{g}(\omega)$.

Compute the curvature and torsion

- From the Frenet-Serret formulae we can deduce

$$\kappa_\gamma(t) = \frac{\|\gamma'(t) \times \gamma''(t)\|}{\|\gamma'(t)\|^3} \tag{1}$$

$$\tau_\gamma(t) = \frac{\gamma'(t) \cdot \gamma''(t) \times \gamma'''(t)}{\|\gamma'(t) \times \gamma''(t)\|^2} \tag{2}$$

- We have γ_{reg} in closed form:

$$\underline{\gamma}_{reg}(t) = (0, t, 0) + \underline{A}_1 \cos\frac{2\pi t}{\ell} + \underline{A}_2 \cos\frac{4\pi t}{\ell} + \underline{B}_1 \sin\frac{2\pi t}{\ell} + \underline{B}_2 \sin\frac{4\pi t}{\ell}$$

where $\underline{A}_i, \underline{B}_i \in \mathbb{R}^3$ are constants depending on $\hat{\gamma}_{reg}$.

- Hence we can calculate the curvature and torsion of γ_{reg} analytically!

Parametrisation by arclength

- The arclength of $\gamma(t) = (x(t), t, z(t))$ is given by

$$s = f(t) := \int_0^t \sqrt{x'(u)^2 + 1 + z'(u)^2}du.$$

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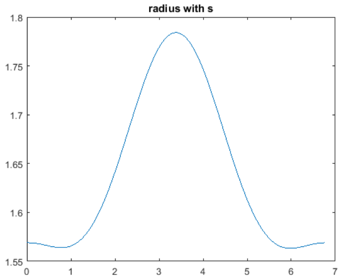
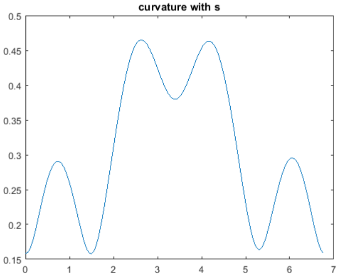
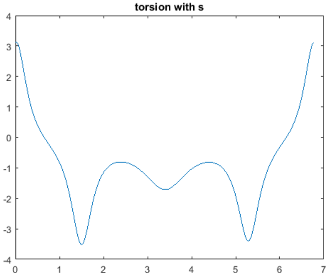
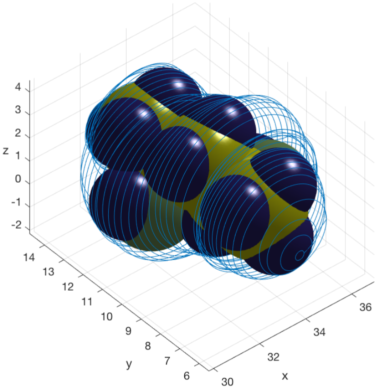
- Compute numerically.


radius with s
1.8
1.75
1.7
1.65
1.6
1.55
0 1 2 3 4 5 6 7

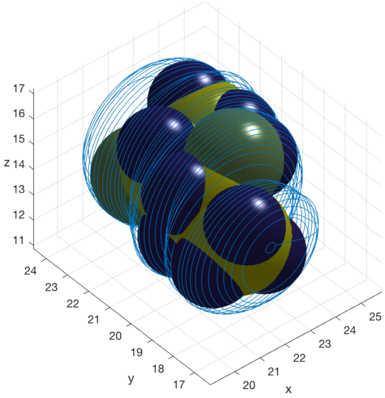

curvature with s
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0 1 2 3 4 5 6 7


torsion with s
4
3
2
1
0
-1
-2
-3
-4
0 1 2 3 4 5 6 7

Question: which molecule gets adsorbed?

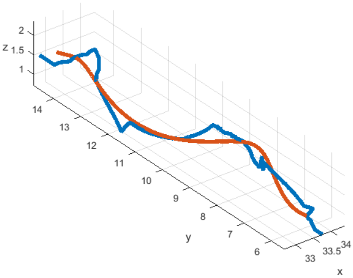


Left 2,4-pentanediol

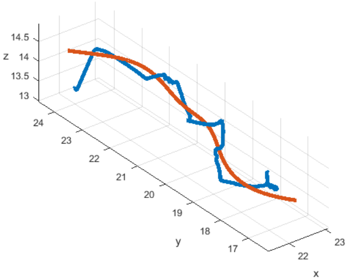


Right 2,4-pentanediol

Question: which molecule gets adsorbed?

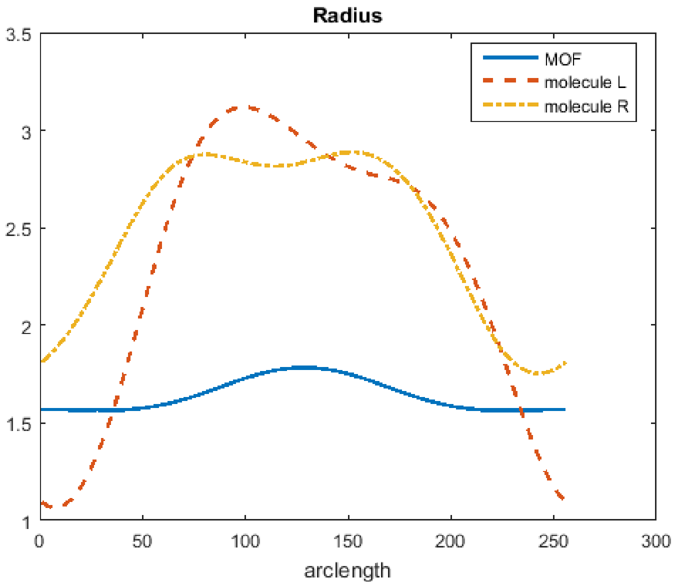


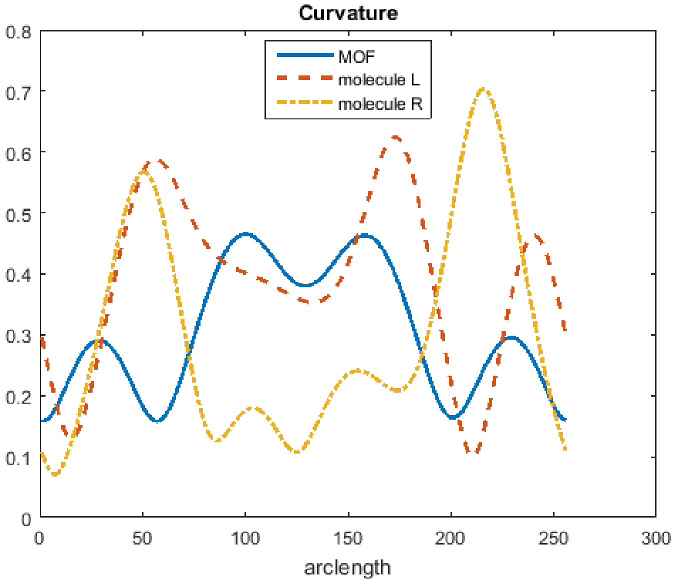
Left 2,4-propanediol



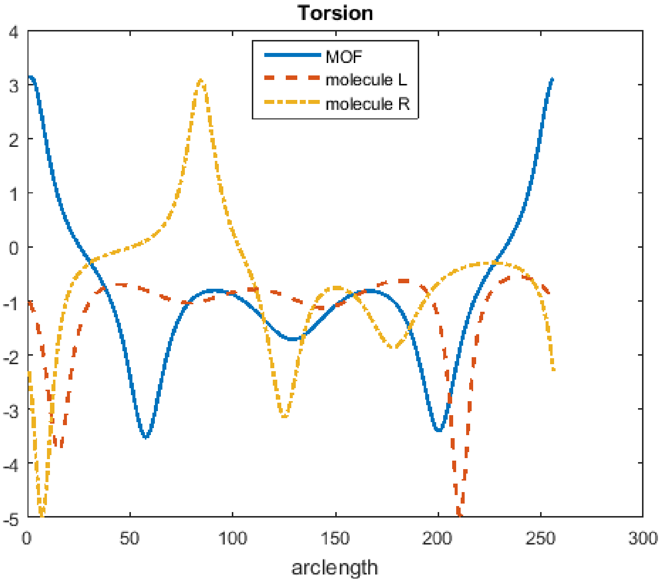
Right 2,4-propanediol

Warning: molecules are not periodic but we imposed a periodic boundary condition!


Radius
3.5
3
2.5
2
1.5
1
0
50
100
150
200
250
300
arclength
MOF
molecule L
molecule R



Curvature
MOF
molecule L
molecule R
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
50
100
150
200
250
300
arclength


Torsion
MOF
molecule L
molecule R
4
3
2
1
0
-1
-2
-3
-4
-5
0
50
100
150
200
250
300
arclength

Questions to consider

- Kinematic vs equilibrium

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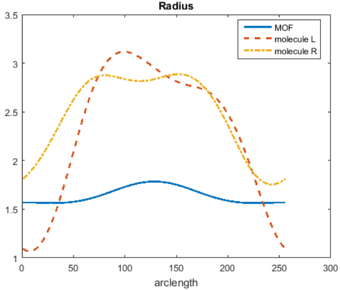
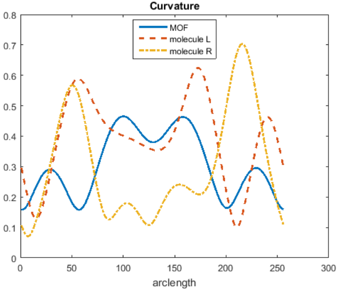
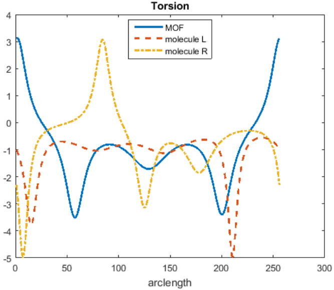
  - **Kinematic problem**: pushing the molecule into the MOF pore
  - **Equilibrium problem**: magically transporting the molecule into the MOF pore and see if it stays in
- Using the radius as tolerance

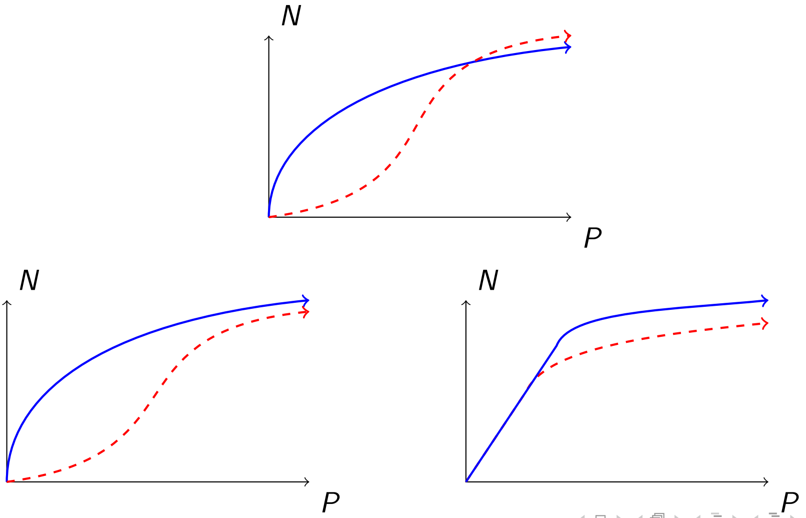

Radius
MOF
molecule L
molecule R
3.5
3
2.5
2
1.5
1
0
50
100
150
200
250
300
arclength


Curvature
MOF
molecule L
molecule R
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
250
300
arclength


Torsion
MOF
molecule L
molecule R
4
3
2
1
0
-1
-2
-3
-4
-5
0
50
100
150
200
250
300
arclength

Adsorption against pressure

3 pairs of molecules: 1,2-pentanediol; 2,4-pentanediol; 1,3-butanediol



Further investigations

- Creating the space of MOFs
- Characterising the spine of the molecule
- Carlos' idea for kinematic fitting as a second screening
- More complex MOFs
- Electrostatic forces