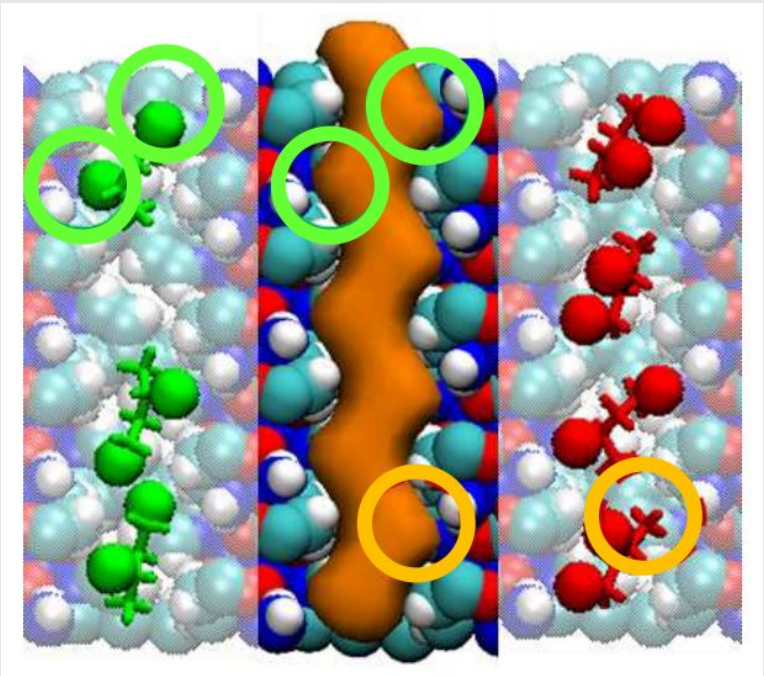
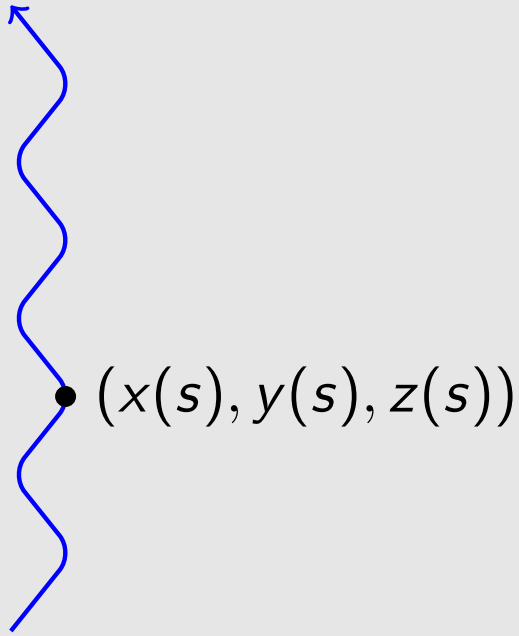
Using Differential Geometry to Classify the Shape of Pores in Metal-Organic Frameworks

Geometry of a pore



Differentiable curve



Geometry of a differentiable curve

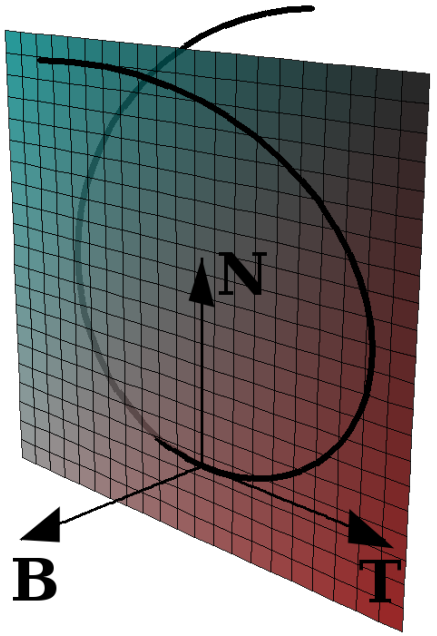
Frenet-Serret formulas

$$\frac{d\mathbf{T}(s)}{ds} = \kappa(s)\mathbf{N}(s) \quad (1)$$

$$\frac{d\mathbf{N}(s)}{ds} = -\kappa(s)\mathbf{T}(s) + \tau(s)\mathbf{B}(s) \quad (2)$$

$$\frac{d\mathbf{B}(s)}{ds} = -\tau(s)\mathbf{N}(s) \quad (3)$$

where κ is the **curvature** and τ is the **torsion**.



Fourier analysis and clustering

Fourier series

Decompose periodic curves into sinusoidal functions, e.g.

$$\kappa(s) = \sum_{n=-\infty}^{\infty} \hat{\kappa}_n e^{2\pi nsi/P}$$

What we are working on

- computing the tube
- creating the space of MOFs
- other geometrical methods

Space of MOFs