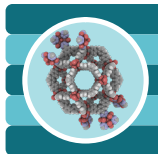


Computational

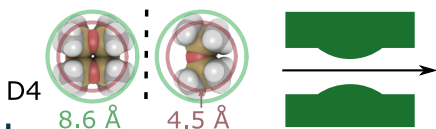


CoRE
MOF
2019



Experimental

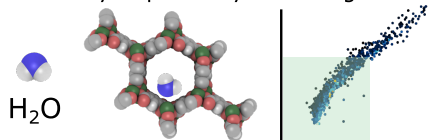
geometric screening



14 000 MOFs

PLD > 6 Å

hydrophobicity screening



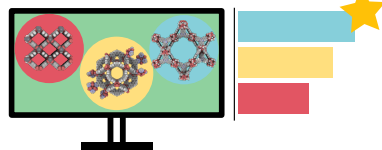
1700 MOFs

$$K_{H^0} < 10^{-5} \text{ mol kg}^{-1} \text{ Pa}^{-1}$$

$$\Delta H_{st^0} < 33 \text{ kJ mol}^{-1}$$

800 MOFs

D4 uptake performance ranking

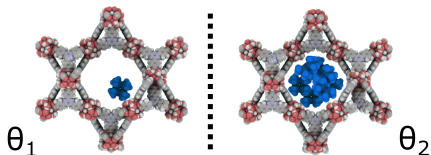


MIL-101(Cr)

benchmark material

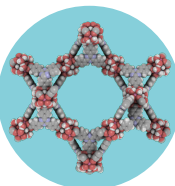
56 MOFs

mechanistic understanding



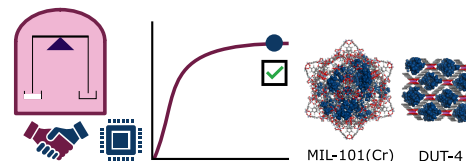
chemical rationale

1 MOF

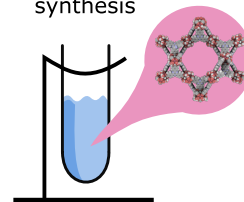


PCN-777

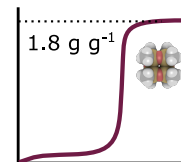
uptake prediction validation



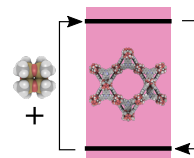
synthesis



D4 sorption



D4 cycling



D4/H₂O stability

