

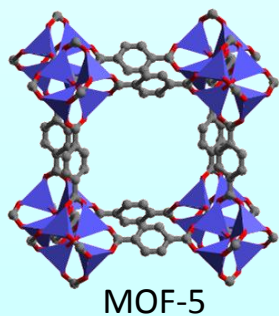
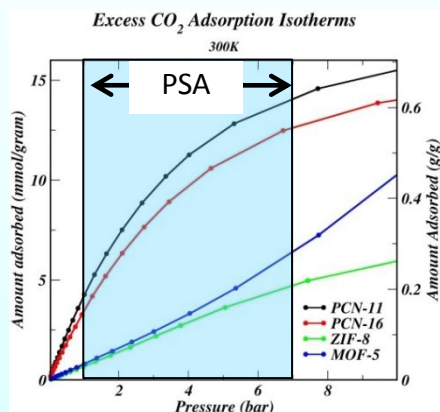
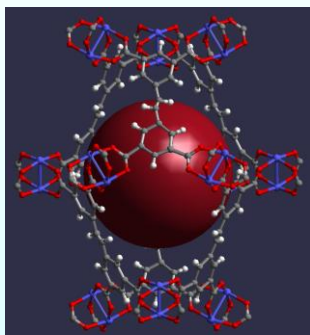
Carbon Capture in Metal Organic Frameworks

Optimum carbon capture and sequestration materials are process dependent

- » Need detailed understanding of CO₂–host material interactions
- » Experiments must take into account industrial applications

Pressure/Vacuum Swing Adsorption

PCN-11

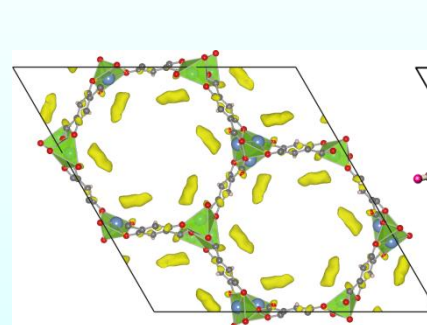


MOF-5

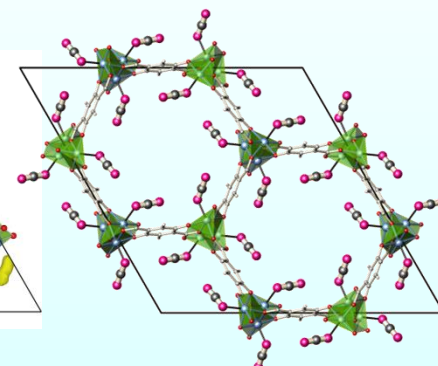
| Material | Saturation (30bar, 300K) | PSA Capacity |
|----------|-----------------------------|-----------------|
| MOF-177* | 40 mmol/g | 6.0 mmol/g |
| MOF-5 | 22 mmol/g | 5.6 mmol/g |
| PCN-11 | 19 mmol/g | 9.9 mmol/g |

* Millward and Yaghi, JACS (2005)

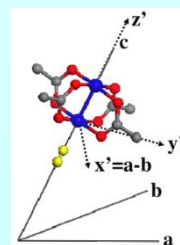
Combined Neutron Scattering and Computational Studies



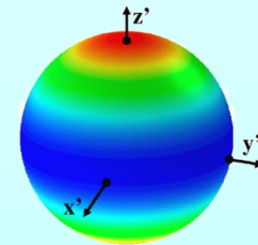
Experimentally determined
CO₂ adsorption sites



DFT Calculated CO₂
adsorption sites



Calculation of the
potential energy
surfaces for
adsorbed species



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