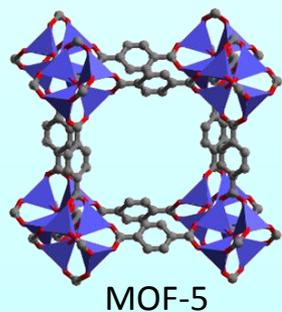
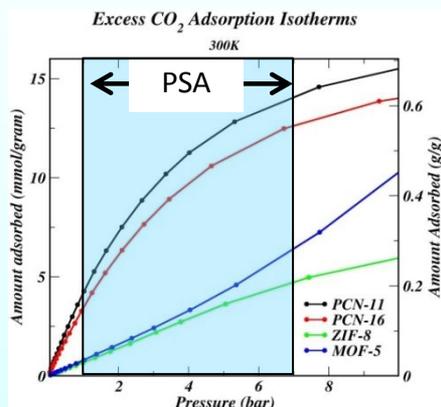
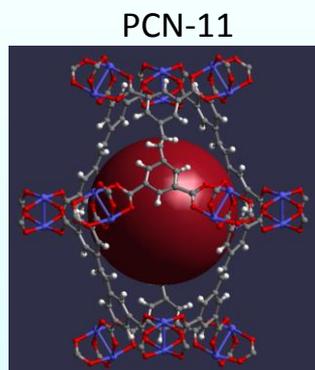


# Carbon Capture in Metal Organic Frameworks

Optimum carbon capture and sequestration materials are process dependent

- » Need detailed understanding of CO<sub>2</sub>-host material interactions
- » Experiments must take into account industrial applications

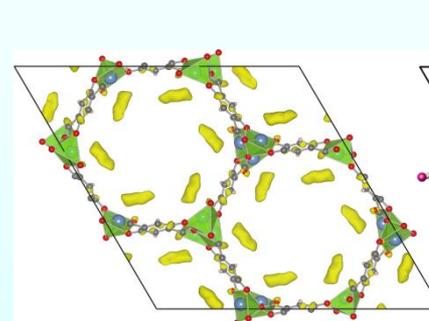
## Pressure/Vacuum Swing Adsorption



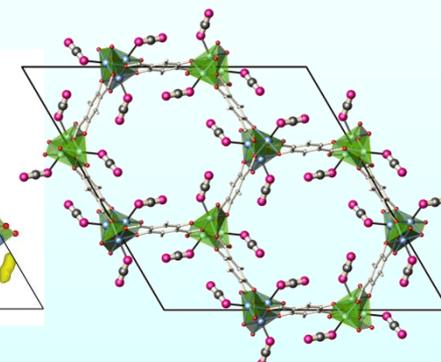
Material	Saturation (30bar, 300K)	PSA Capacity
MOF-177*	40 mmol/g	6.0 mmol/g
MOF-5	22 mmol/g	5.6 mmol/g
PCN-11	19 mmol/g	9.9 mmol/g

\* Millward and Yaghi, JACS (2005)

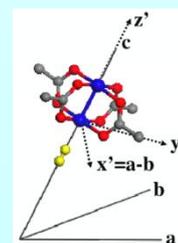
## Combined Neutron Scattering and Computational Studies



Experimentally determined CO<sub>2</sub> adsorption sites



DFT Calculated CO<sub>2</sub> adsorption sites



Calculation of the potential energy surfaces for adsorbed species

