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Atomic-scale understanding of CO2 adsorption processes in metal-organic framework (MOF) materials using neutron scattering and ab initio calculations

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The dependence of the industrialised world on fossil-fuel energy generation technologies and consequent increase in atmospheric CO2 concentrations has been blamed for emerging adverse climate effects, including an increase in global mean temperatures [1]. Until renewable, carbon-free energy sources can be efficiently harnessed to meet the world's energy needs, interim measures are sought to suppress the atmospheric release of CO2 from traditional coal and natural gas combustion processes. Microporous materials such as zeolites and metal-organic frameworks (MOFs) are therefore being investigated for the separation and capture of CO2 at various stages of the combustion cycle.

MOFs represent one of the most promising classes of materials for this application, offering unrivalled tunability of structural and chemical characteristics via the substitution of metals and choice and functionalisation of ligands [2]. In order for a MOF to be rationally tuned for improved performance, the nature of the interactions between the host framework and guest molecules must be well-understood at the atomic level. Our research targets this detailed understanding of MOFs using neutron scattering and computational methods.

We are currently investigating several MOFs which display unexpected sorption properties such as "reverse sieving" – that is, selectively absorbing larger gas molecules while rejecting smaller ones – and unusual lattice expansion effects. Using in situ diffraction to locate the preferred binding sites of guest molecules in the framework, inelastic neutron scattering to probe system dynamics, and density functional theory-based molecular dynamics simulations to validate and interpret our experimental results, we are able to gain detailed information about the mechanisms of gas uptake and diffusion in these exciting new MOF materials.

[1] S. Solomon, G.K. Plattner et al., Proc. Natl. Acad. Sci. USA **106** (2009) 1704-1709.

[2] G.J. Kearley & V.K. Peterson (eds.), Neutron Applications in Materials, Springer (2015).

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