Neutron Diffraction and In Situ Gas-Loading Investigations of Functional MOFs for Energy-Relevant Gas Separations

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Intense research is currently directed towards realising metal-organic frameworks (MOFs) for industrially-applied gas separation and storage due to their unique structural properties, including: robustness; thermal and chemical stability; unprecedented internal surface area; and high void volume. A particular focus of current research is the development of MOFs for the separation of CO_2 from the other components of flue gas in fossil-fuelled power plants.

The use of NPD to study gas adsorption in framework materials is a relatively new but growing field. Structural measurements, which show the arrangement of both the host and guest, allow derivation of the nature of the host-guest interaction, and the host's response to the guest. The capability to perform these measurements, with accurate gas dosing and temperature control, has recently been realised at ANSTO's Bragg Institute.[1] Using these techniques, we have investigated the adsorption mechanisms of a number of gases in selected new and established MOFs that display impressive selectivity for specific gases. The location and orientation of industrially-relevant gases including D_2, O_2, CO_2, and CD_4 within their crystal structures provide insights into the modes of binding, which will help to tune the materials' performance and benefit the design and development process for the next generation of materials.

[1] Bloch, E. D.; Murray, L. J.; Queen, W. L.; Chavan, S.; Maximoff, S. N.; Bigi, J. P.; Krishna, R.; Peterson, V. K.; Grandjean, F.; Long, G. J.; Smit, B.; Bordiga, S.; Brown, C. M.; Long, J. R. J. Am. Chem. Soc. 2011, 133, 14814.