In-situ Gas Adsorption Studies at Modest and Extreme Pressures within Metal Organic Frameworks

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In recent years the development of new methods of storing, trapping or separating light gases, such as CO_2, CH_4 and CO has become of utmost importance from an environmental and energetic viewpoint. Porous materials such as zeolites and porous organic polymers have long been considered good candidates for this purpose. More recently, metal organic frameworks (MOFs) have attracted further interest with many aspects of their functional and mechanical properties investigated. The porous channels found in MOFs are ideal for the uptake of guests of different shapes and sizes, and with careful design they can show high selectivity for particular species from a mixture.[1] Adsorption properties of MOFs have been thoroughly studied,[2] however obtaining in depth 'structural' insight into the adsorption/desorption mechanism is not so common place. For example, out of *ca.* forty thousand published framework structures there are less than 60 entries in which CO_2 molecules have been experimentally located within the pores.[3]

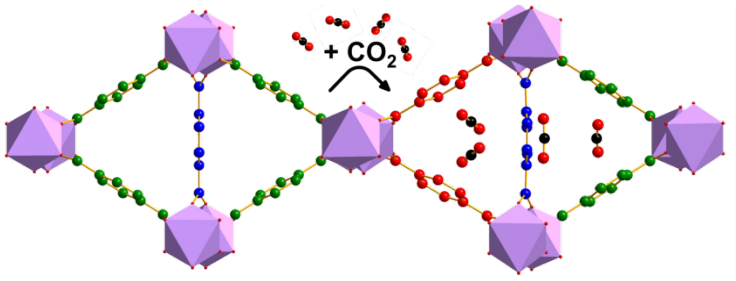

Fig. 1 Structure of Sc_2BDC_3 before and after uptake of CO_2 guest molecules.

In this study, we present a series of high-pressure gas and diamond anvil cell studies conducted on beamline I19 at Diamond Light Source. Here, we have studied the inclusion of a variety of gas molecules on the microporous scandium framework, Sc_2BDC_3 (BDC = benzene-1,3-dicarboxylate, Fig. 1) and its amino functionalised derivative $Sc_2(BDC\text{-}NH_2)_3$ ($BDC\text{-}NH_2$ = 2-aminobenzene-1,3-dicarboxylate).[4,5] During these studies, not only has it been possible to reveal the different adsorption sites for CO_2, CH_4 and CO in both frameworks but also the change in uptake as a function of increasing gas pressure. Additionally, gas mixtures have also been investigated, including CO_2/CH_4 with various compositions, revealing selectivity within the MOF pores. With atomistic resolution of the guest molecules within the pores, it is now possible to recognise the interactions that facilitate greater uptake for particular guest molecules in detail, and therefore understand how to optimise and develop MOFs for more effective gas adsorption properties.

References

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