Poster Presentations

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Due to the growing interest in carbon storage, gas separation, gas purification and hydrogen fuel cells, the study of materials which are capable of these functionalities has become increasingly important. Crystallography can offer valuable information about gas interactions with the framework and the information gained can be used to design new materials. I19 beamline at Diamond Light Source has further developed the ‘gas cell’ which can be used to observe the removal and uptake of gas or solvent molecules in-situ within a single crystal. Framework materials often have large pours which are filled with disordered molecules, and hence the diffraction drops off at higher angles. Therefore synchrotron radiation offers the X-ray flux required to achieve atomic resolution. The high flux also offers the advantage of relatively quick data collection for complete data sets (20 to 40 min) allowing the uptake of gas or solvent molecules to be measured on faster time-scales. With our current design we achieve a vacuum of \( \frac{1}{10} \) mbar and pressure of 15 bar with selected gases. Gas can also be flowed over the sample with flow rates ranging from 0 to 100 ml/min. There are several gas cells which are interchangeable so that more than one process can be measured simultaneously. The current setup has been utilised successfully to crystallographically monitor the increase in gas absorption, the gas location within the pours and also the gas selectivity of mixture of gases.