Quick sorption analysis for CO_2 adsorption on isostructural metal-organic frameworks with various 3d metals

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Introduction

Novel metal-organic frameworks (MOFs) are being produced at a high rate for application in gas separation, storage and catalysis. The Barbour group has the capabilities to study porous materials by single crystal (SC) and powder X-ray diffraction (PXRD) experiments.[1]

The instrument presented serves the purpose to determine the feasibility of quantitative sorption studies.

Method

The instrument is controlled by a RaspberryPi and consists of a sample chamber (S, Figure 1) with an electronic pressure sensor separated from the reservoir chamber (R) by an electronically controlled valve (V). The reservoir is equipped with an analogue 10 bar pressure gauge to monitor the input pressure. Aside from the inlet to the reservoir, the system is completely controlled by the software (Figure 2).

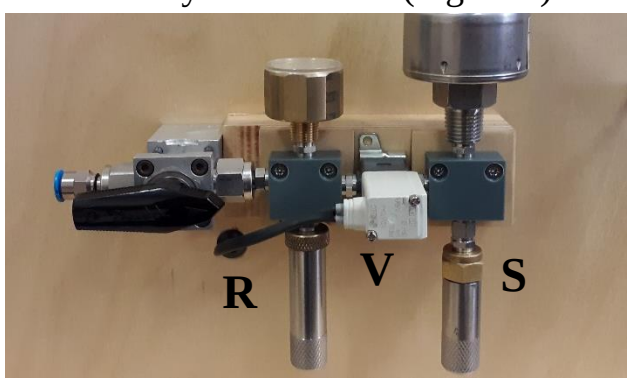

Figure 1 Hardware setup

Isostructural MOFs with Zn, Cu, Ni, Co and Mn were crystalized and their structures obtained from XRD (Figure 3). The bulk samples were added to the sample chamber and evacuated before loading it up with CO_2 up to 5 bar. The pressure was monitored continuously. The graph of the pressure over time was plotted at the end.

Reference

[1] P. Lama, L. J. Barbour, *J. Am. Chem. Soc.* **2018**, 140, 2145-2150.

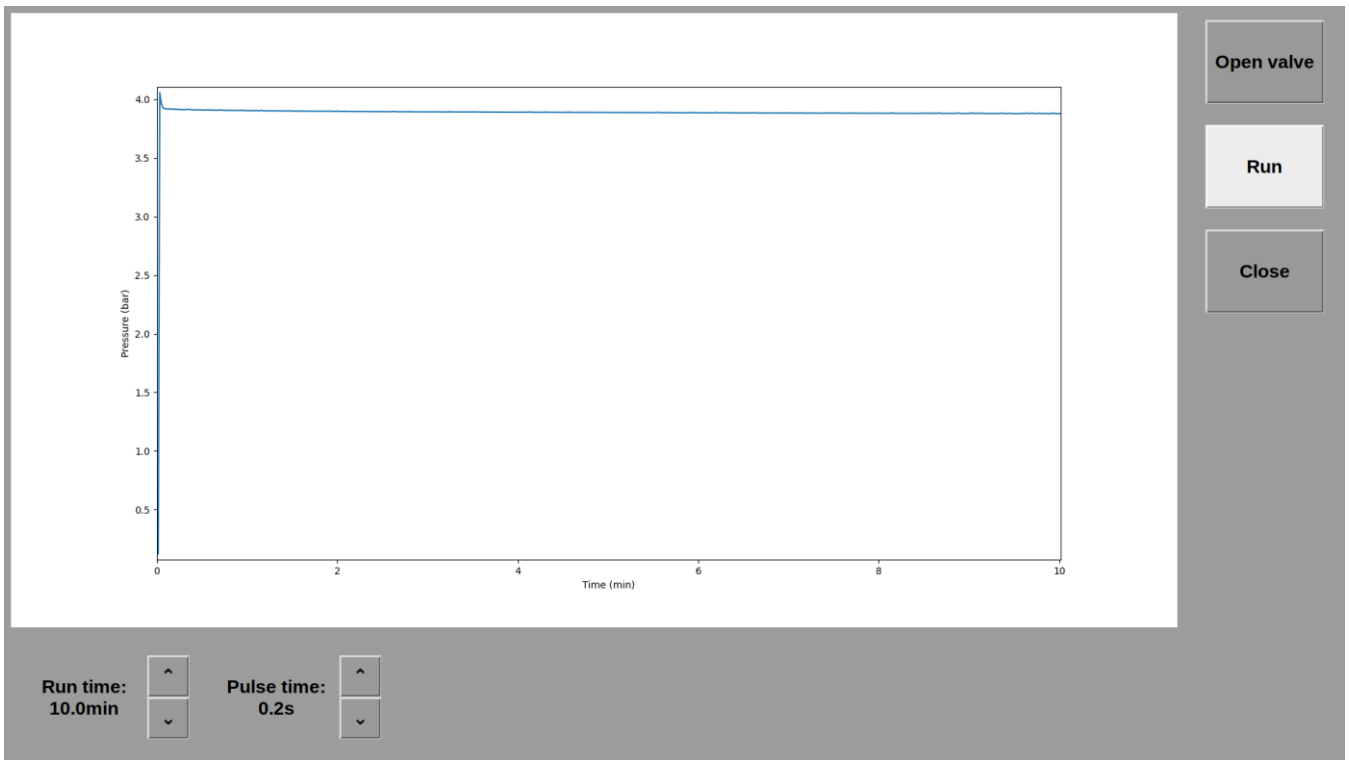

Figure 2 Screen Capture of a Zn MOF Sorption run with CO_2 at 4 bar for 10 minutes.

Results & Discussion

A positive result would present as a gradual decrease in pressure over time as the sample adsorbs CO_2, thus reducing the overhead pressure in the sample chamber.

The results with the different metals suggest that all the analogues retained the CO_2 sorption capability (gradually decreasing pressure, Figure 4). Thus, they can be further studied by quantitative means.

The jumps in the data of around 50 mbar, seemingly due to temperature variations.

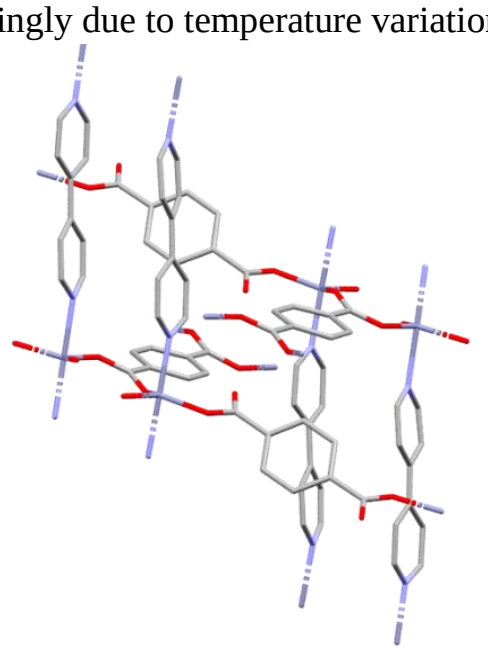

Figure 3 Crystal structure of Zn MOF.

The data for the Zn MOF under different pressures (0 to 5.5 bar) suggest that CO_2 was only adsorbed above 3 bar. This insight can guide the development of quantitative sorption experiments.

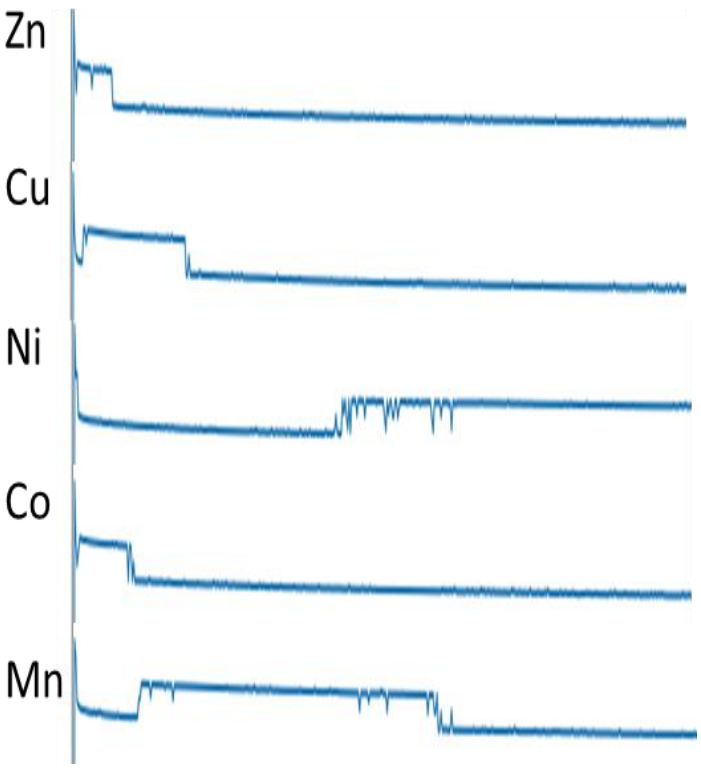

Figure 4 Results with different metals under 5 bar CO_2 pressure.

Conclusions

The MOF analogues showed potential for CO_2 sorption capability and can thus be further investigated by more elaborate techniques.

Improvements are being made to increase the sensitivity and thermal stability of the instrument. It can, however, already help identify samples that seem feasible for in-depth sorption experiments.

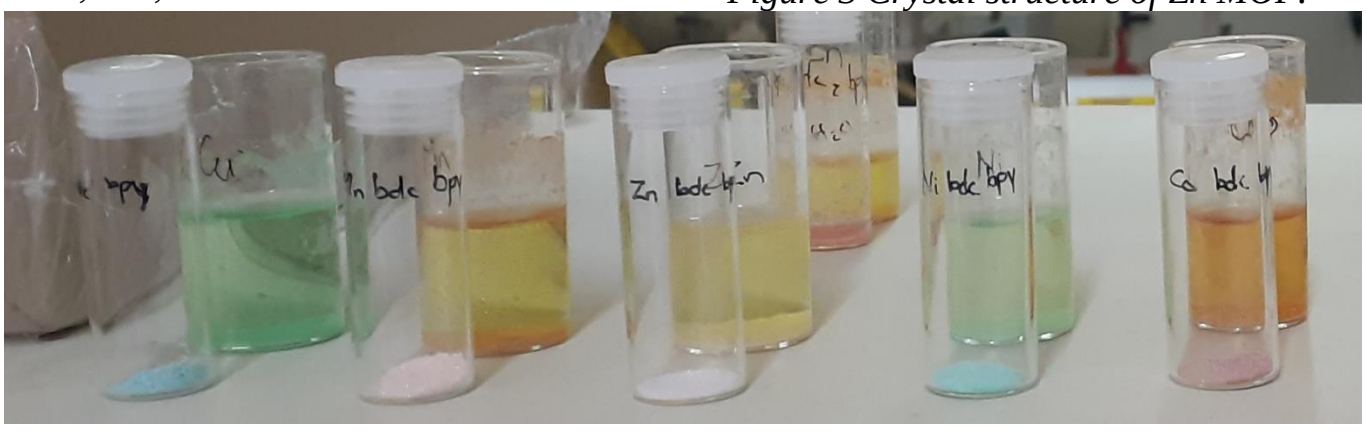

Figure 5 Samples used for the experiments.