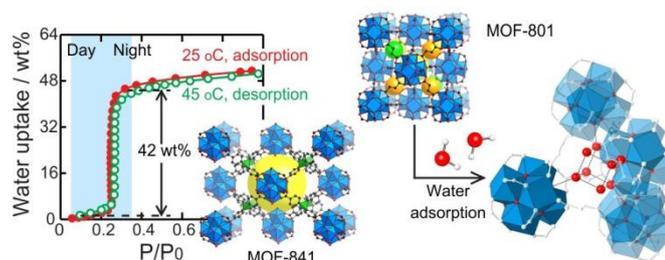


B-T-011-en

## Repeated performance evaluation of water vapor adsorption and desorption for PCP/MOF (porous metal organic framework)

### Introduction

The adsorption of water by porous materials is important for many applications requiring capture and release of water. Some of the key applications include dehumidification, thermal batteries, and the delivery of drinking water to remote areas (1). Generally, there are three key considerations when designing adsorbent materials suitable for water storage, including:



- 1) Pore filling or condensation of water into the porous materials must occur at low relative pressure ( $P/P_0$ ) or relative humidity (RH) and exhibit a steep uptake behaviour.
- 2) The water uptake capacity of the material must be high for maximum delivery of water and simple adsorption/desorption processes for energy efficiency.
- 3) High adsorption/desorption cycling performance and water stability of the material.

Metal-Organic Frameworks (MOFs) were examined for their water adsorption properties in this application note.

A variety of zirconium-based MOFs were designed to meet the three criteria mentioned above. Their water adsorption behaviours were examined by using a BELSORP-aqua3 at the University of California, Berkeley (USA).

Key words: MOF, Water adsorption, Capture and release of atmospheric water, Cycle performance

### Experiment

Water vapor adsorption isotherms of zirconium-based MOFs and zeolite 13X at 25 °C were measured on a BELSORP-aqua3 (present model: BELSORP MAX X HT) volumetric vapor adsorption analyser. User-friendly measurement software enables unattended cycle performance testing over five consecutive cycles. The sample was evacuated for 2 h at 25 °C between cycles. It can also measure 3 samples simultaneously, enabling high-throughput measurements.

### Results and Discussion

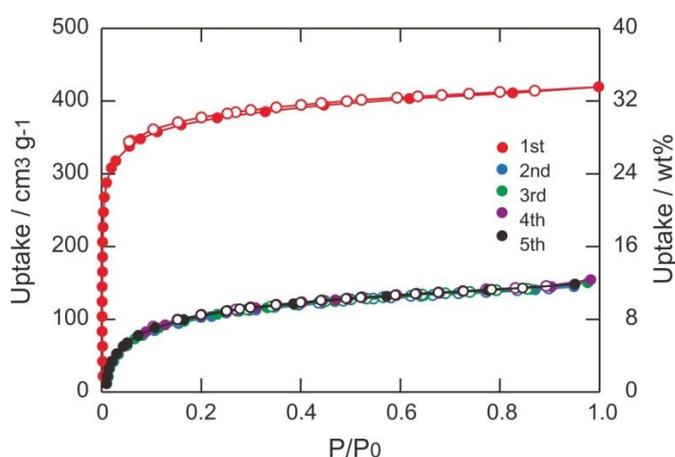


Fig. 1. Cycle performance of water uptake in Zeolite 13X at 25 °C

Zeolites are commercially used to capture moisture in electric dehumidifiers because of their ability to adsorb water at very low relative pressures. However, due to the strong interaction between zeolites and water molecules, it is necessary to heat the material up to 300 °C to desorb the adsorbed water molecules from the pores. This regeneration process requires high energy input. Therefore, zeolites are not ideal materials for applications related to water capture and release. This can be observed in Fig. 1 where the Zeolite sample showed significantly higher water adsorption capacity for the first cycle whereas it failed to regain the same adsorption capacity for successive cycles after regeneration at room temperature.

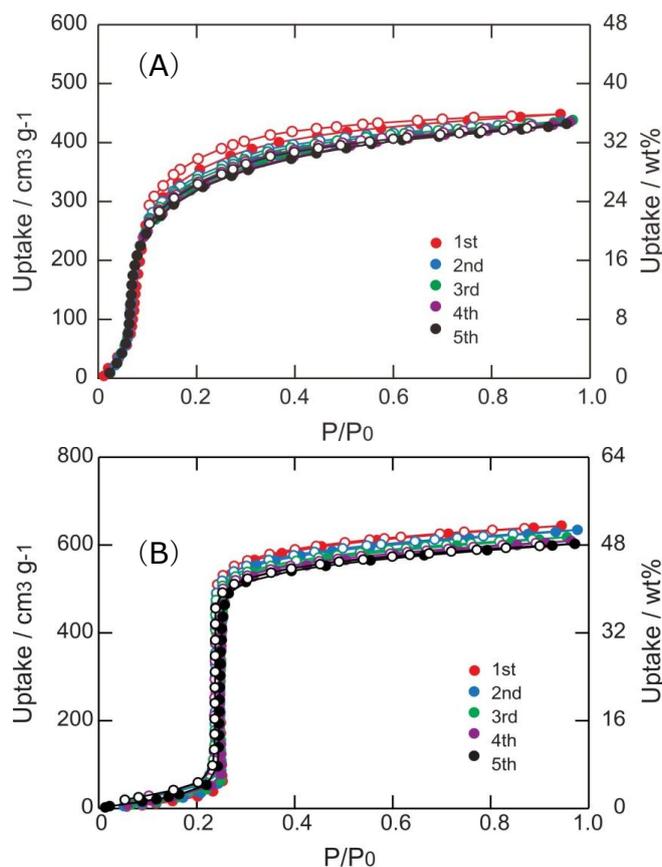


Fig. 2. Cycle performance of water uptake in MOF-801-P (A) and MOF-841(B)

MOFs can also be used for water harvesting applications to capture, store and release of atmospheric water in remote desert areas where drinking water is scarce. In such areas, typical summer daytime temperature and relative humidity (RH) are 40 °C and 5%, which drastically changes at night to 25°C and 35%. Under such conditions, porous materials can capture water between 5% and 35% RH (i.e.  $P/P_0 = 0.05-0.35$ ), then water vapor in the air can be condensed. Considering that MOF-841 took up 44% of water at  $P/P_0 = 0.3$ , MOF-841 has great potential to capture, store and release of the atmospheric water.

## Conclusion

Zirconium-based MOFs demonstrate high performance for the applications requiring capture, store and release of water. Through the water vapor adsorption instrument, the uptake of water by MOFs is evaluated and their cyclability was effectively studied in this application note. However, uptake capacity and cyclic stability also depends on the defects in the crystal structure of the MOFs (2).

## Reference

- (1) Furukawa, H. et al. *J. Am. Chem. Soc.* **136**, 4369–4381 (2014).
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Microcrystalline powder sample of MOF-801-P (Fig.2 (A)) and MOF-841 (Fig.2 (B)) showed high performance based on the three criteria mentioned in the introduction. The water uptake in these MOF materials was steep and the maximum uptake was nearly constant even after five consecutive cycles. This clearly indicates that these MOF materials show strong interaction with water and at the same time, can be easily regenerated under mild conditions.

In order to utilize MOFs as heat exchangers for automobiles (so-called thermal batteries), water capture at low relative pressures ( $P/P_0 < 0.1$ ) is desirable as it reduces the need to incorporate compressors or to raise the evaporation temperature for the adsorption/desorption cycles. In that regard, MOF-801-P is a good candidate to be used in advanced thermal batteries.