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**<Supplementary Information>**

# Selective separation of Xe/Kr and adsorption of water in a microporous hydrogen-bonded organic framework

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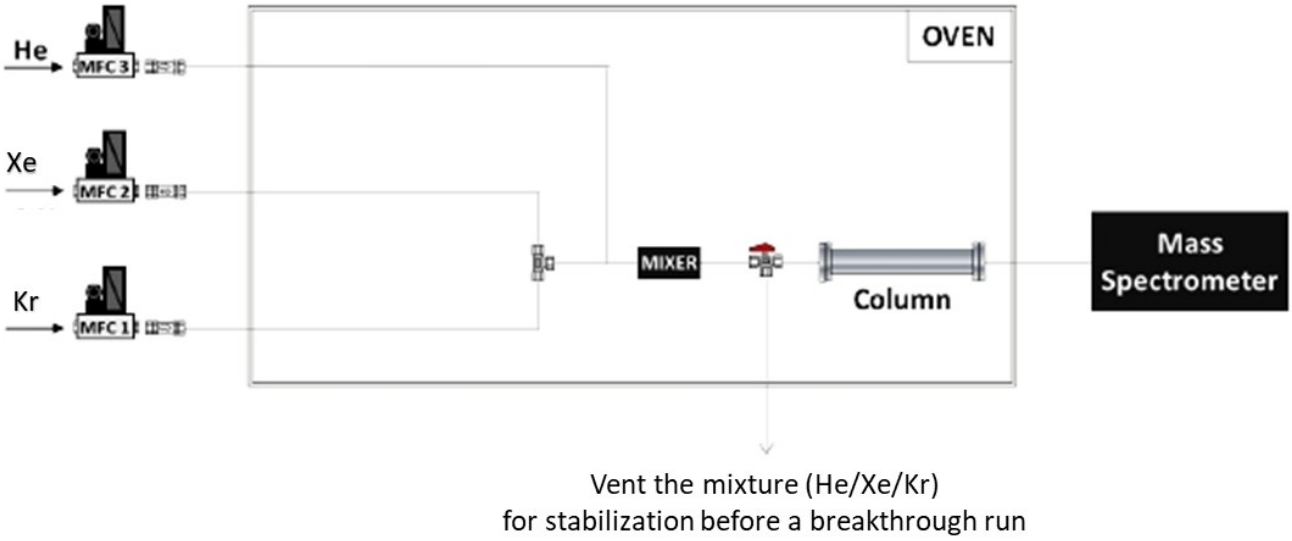


**Scheme S1** A schematic diagram of the dynamic breakthrough experimental setup.

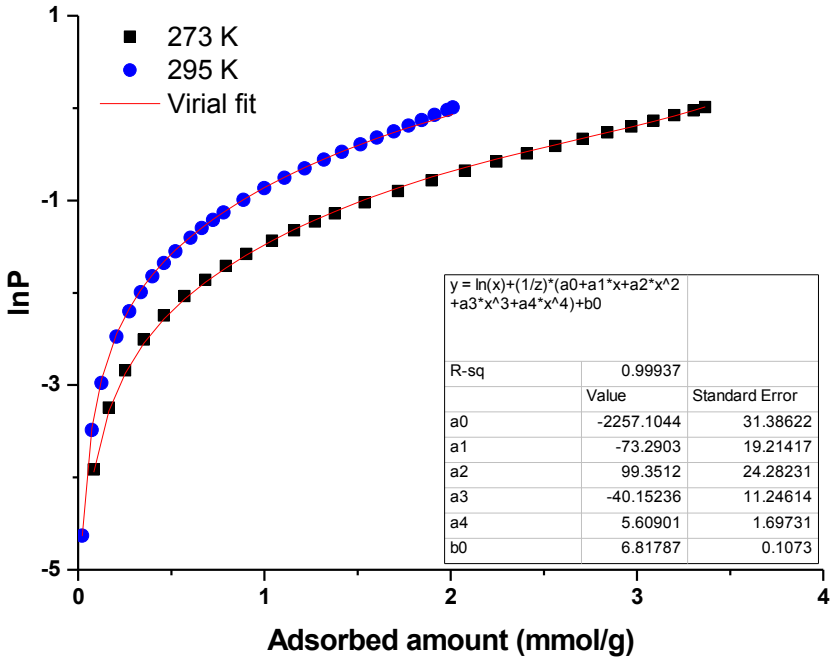


**Fig. S1** Virial fitting obtained from Xe adsorption isotherms at 273 K and 295 K. Calculated parameters were given in the inset table.

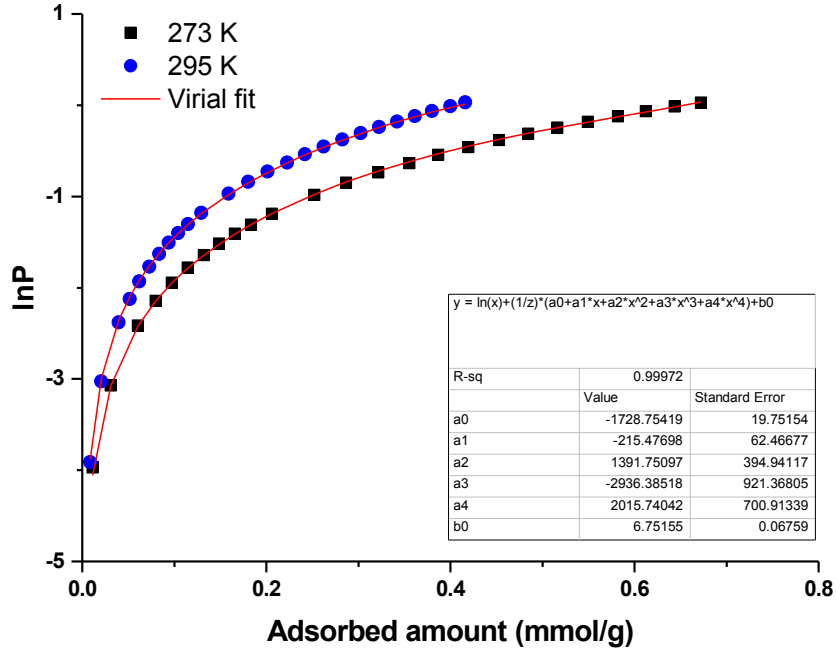


**Fig. S2** Virial fitting obtained from Kr adsorption isotherms at 273 K and 295 K. Calculated parameters were given in the inset table.

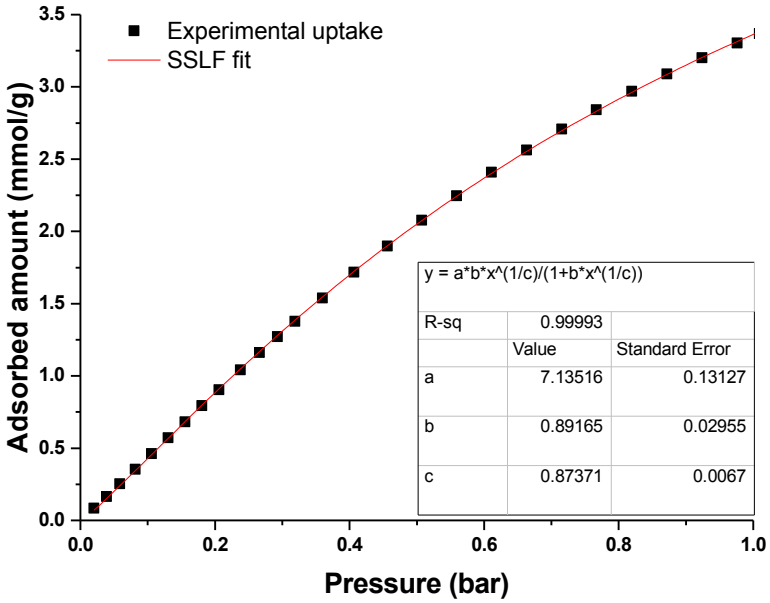


**Fig. S3** Single site Langmuir-Freundlich (SSLF) fitting obtained from the Xe adsorption isotherm at 273 K. Calculated parameters were given in the inset table.

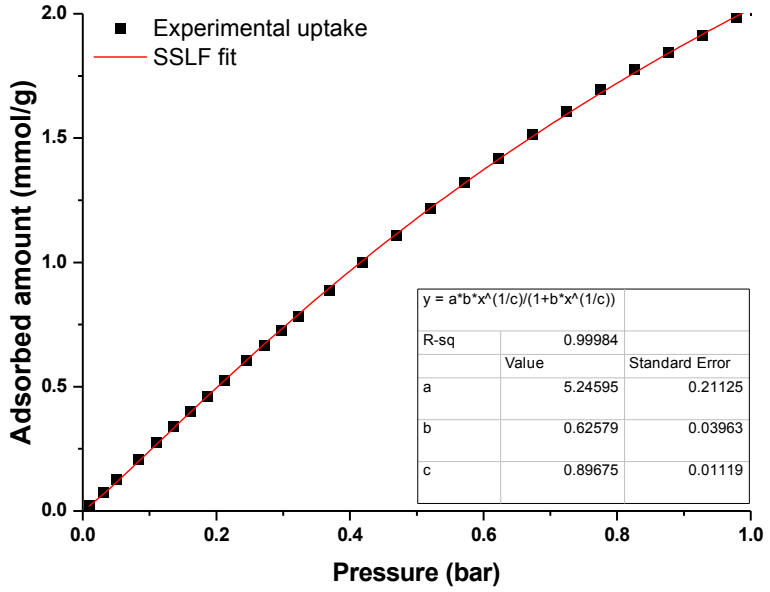


**Fig. S4** Single site Langmuir-Freundlich (SSLF) fitting obtained from the Xe adsorption isotherm at 295 K. Calculated parameters were given in the inset table.

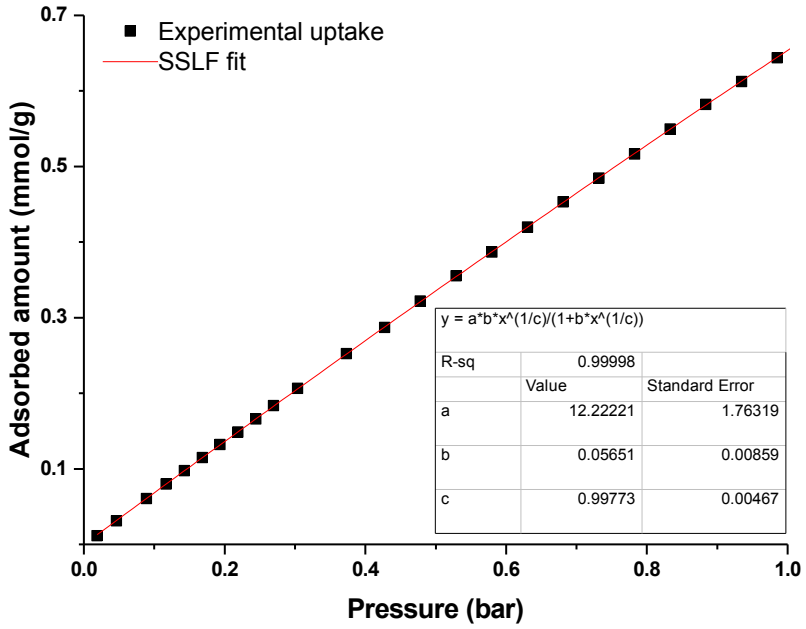


**Fig. S5** Single site Langmuir-Freundlich (SSLF) fitting obtained from the Kr adsorption isotherm at 273 K. Calculated parameters were given in the inset table.

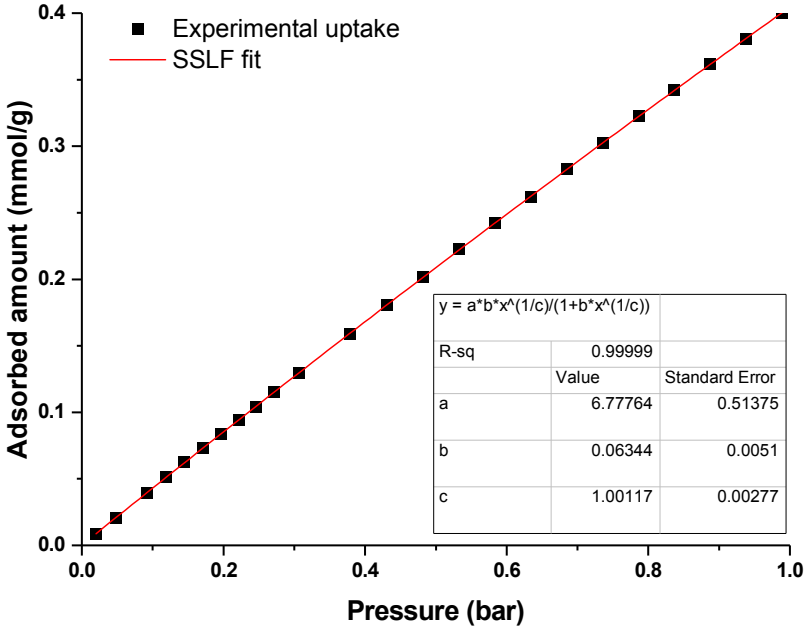


**Fig. S6** Single site Langmuir-Freundlich (SSLF) fitting obtained from the Kr adsorption isotherm at 295 K. Calculated parameters were given in the inset table.

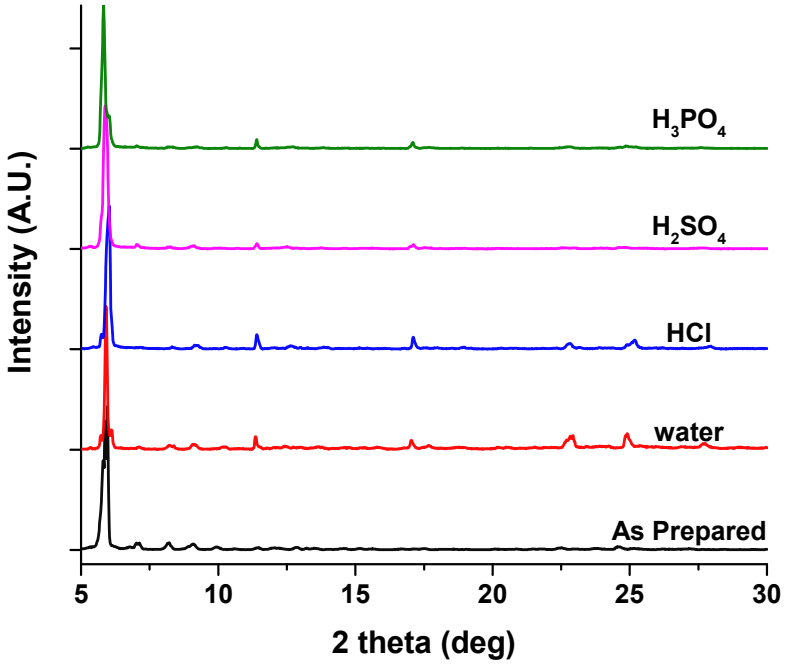


**Fig. S7** Powder X-ray diffraction patterns of as-prepared HOF-BTB crystals in water, 1 N HCl, 1 N $H_2SO_4$, and 1 N $H_3PO_4$ solutions for one month. Small shifts in the diffraction peaks could be attributed to incomplete drying of the samples.

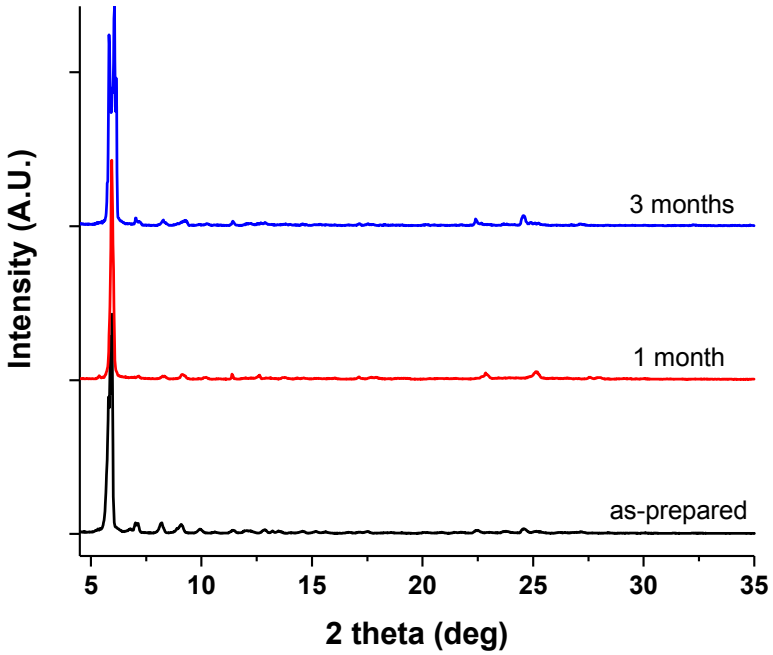


**Fig. S8** Powder X-ray diffraction patterns of as-prepared HOF-BTB crystals in water for one month and three months.

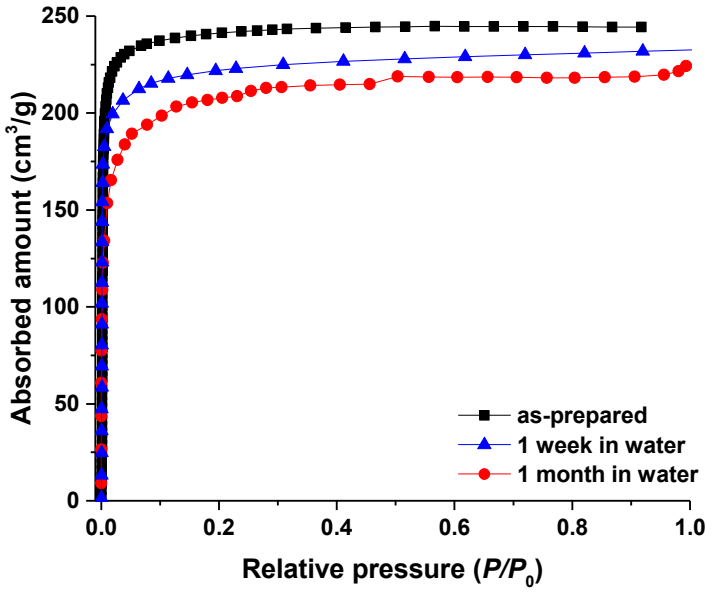


**Fig. S9** $N_2$ adsorption isotherms of HOF-BTB crystals after immersing in water for one week and one month. The $N_2$ isotherm for the as-prepared HOF-BTB sample was shown for comparison.

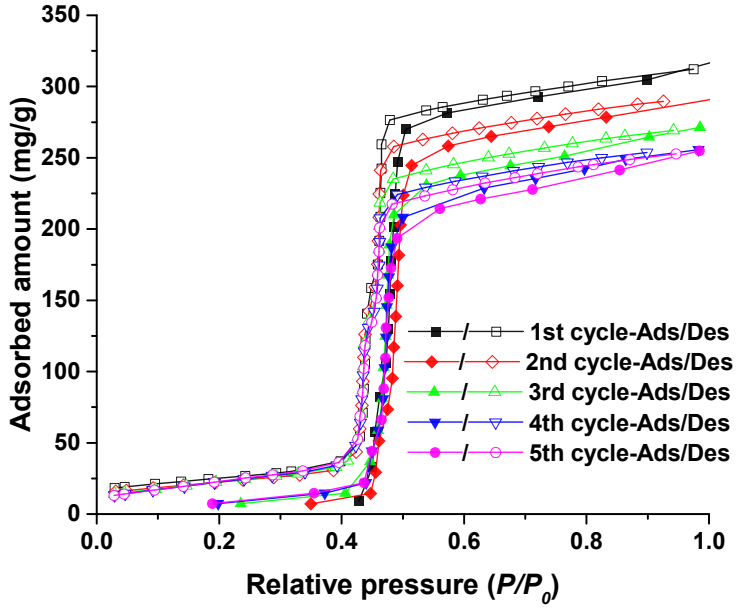


**Fig. S10** Water vapor adsorption/desorption isotherms up to 5 cycles at 298 K.