Electronic Supplementary Information for

Tailoring the Water Adsorption Properties of MIL-101 Metal-Organic Frameworks by Partial Functionalization

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General Procedures

All chemicals and solvents used in the syntheses of compounds were of reagent grade and used without further purification. $Cr(NO_3)_2 \cdot 9H_2O$, $CrCl_3$, $SnCl_2$, tetramethylammonium hydroxide (TMOH), benzene-1,4-dicarboxylic acid (H_2BDC), 1,5-dihydroxynaphthalene, bromine, ethyl isocyanate (Et-NCO), maleic anhydride, 1,3-propanesultone, and benzene-1,2,4-tricarboxylic acid ($H_3$2-BTC) were purchased from Sigma-Aldrich. Powder X-ray diffraction (PXRD) data were collected on a Rigaku MiniFlex diffractometer with CuKα radiation (λ = 1.5418 Å). Thermogravimetric analyses (TGA) were carried out using a Scinco TGA-S1000 thermal analysis system under air with a temperature-increasing rate of 5 °C/min. NMR spectra were obtained on a Bruker 400 MHz NMR spectrometer. The N_2 adsorption isotherms were measured using the standard volumetric procedure on a BELSORP-mini (BEL-Japan, INC.). All samples were activated under vacuum at 180 °C for 6 h before the sorption measurements.

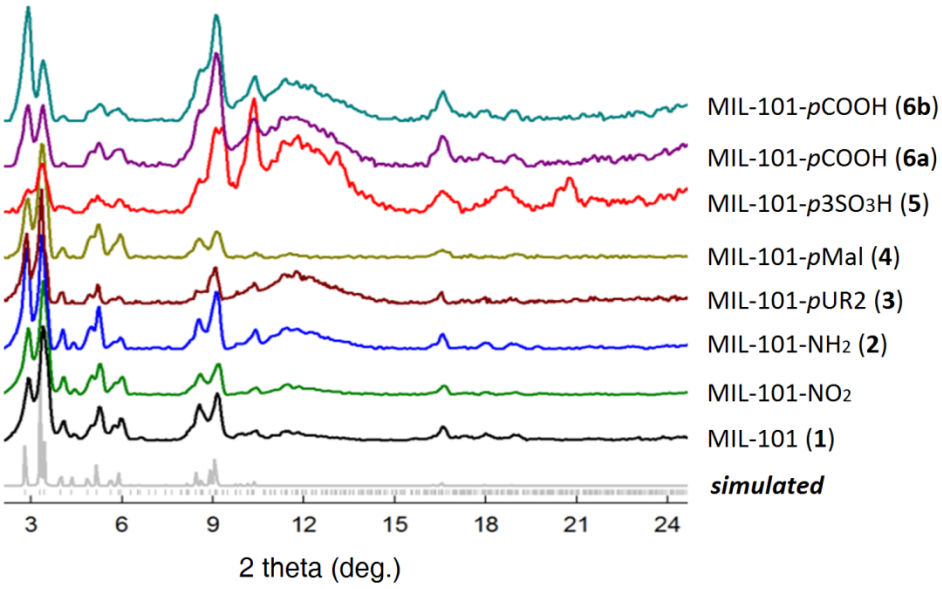

Fig. S1 PXRD patterns of MIL-101 and its derivatives. The broad peaks at 2θ = 12°are due to the coated silicon grease on sample holders.

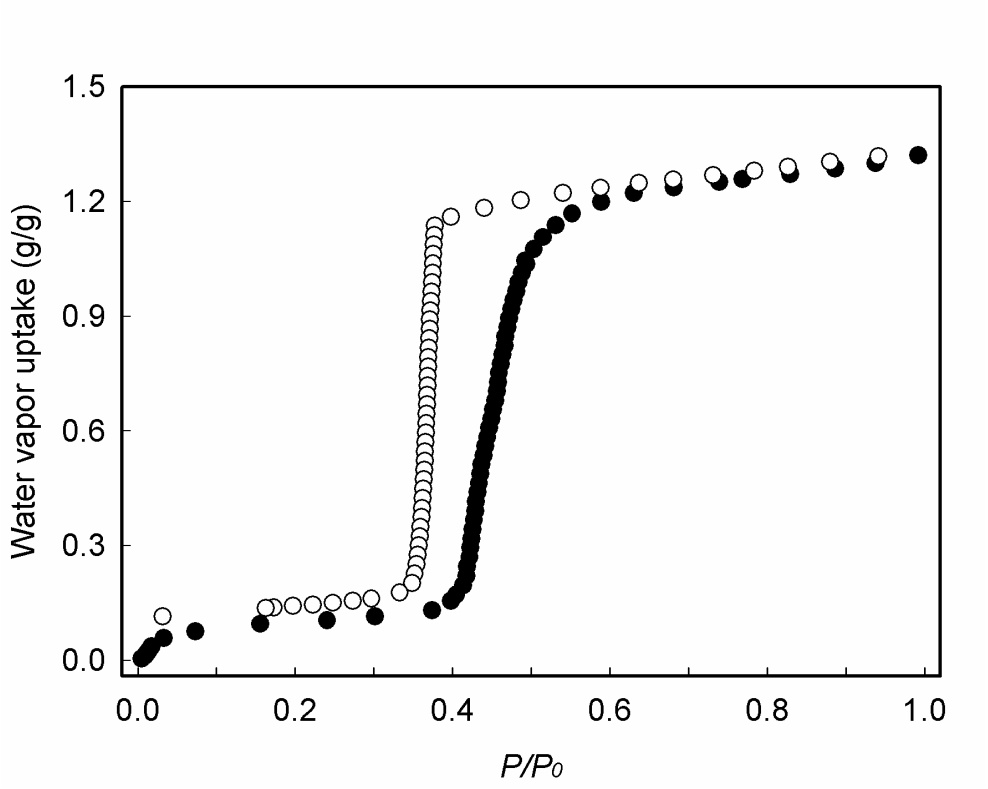

Fig. S2 Water vapor sorption isotherm of MIL-101 (**1**). Filled and empty symbols correspond to adsorption and desorption points, respectively.

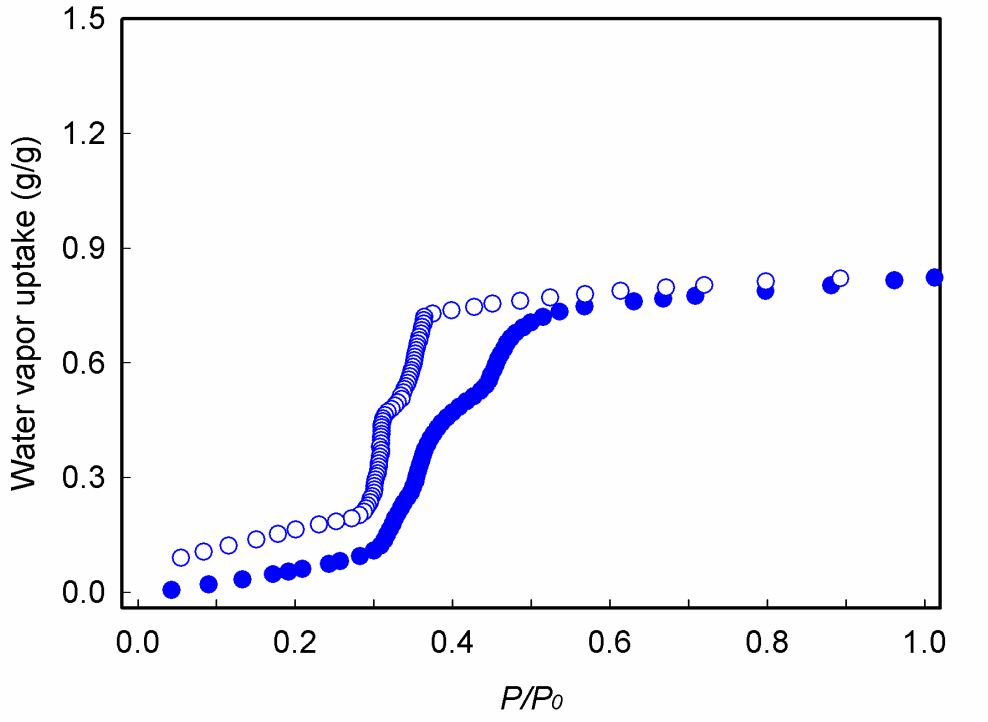

Fig. S3 Water vapor sorption isotherm of MIL-101-NH_2 (**2**).

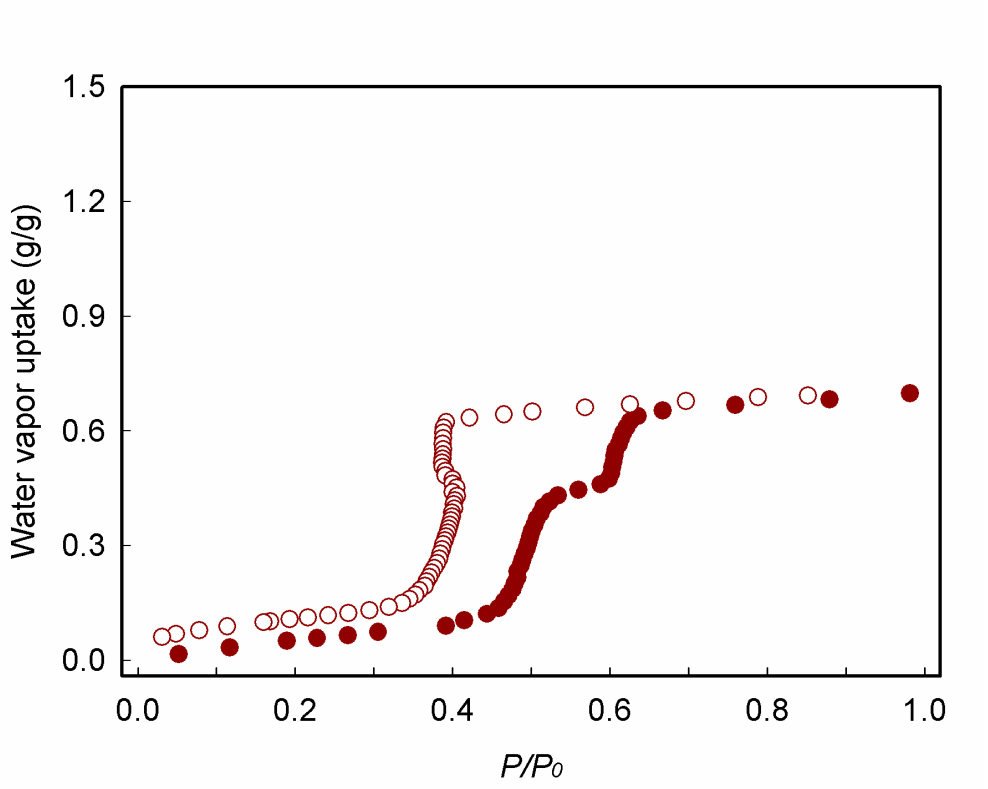

Fig. S4 Water vapor sorption isotherm of MIL-101-*p*UR2 (**3**).

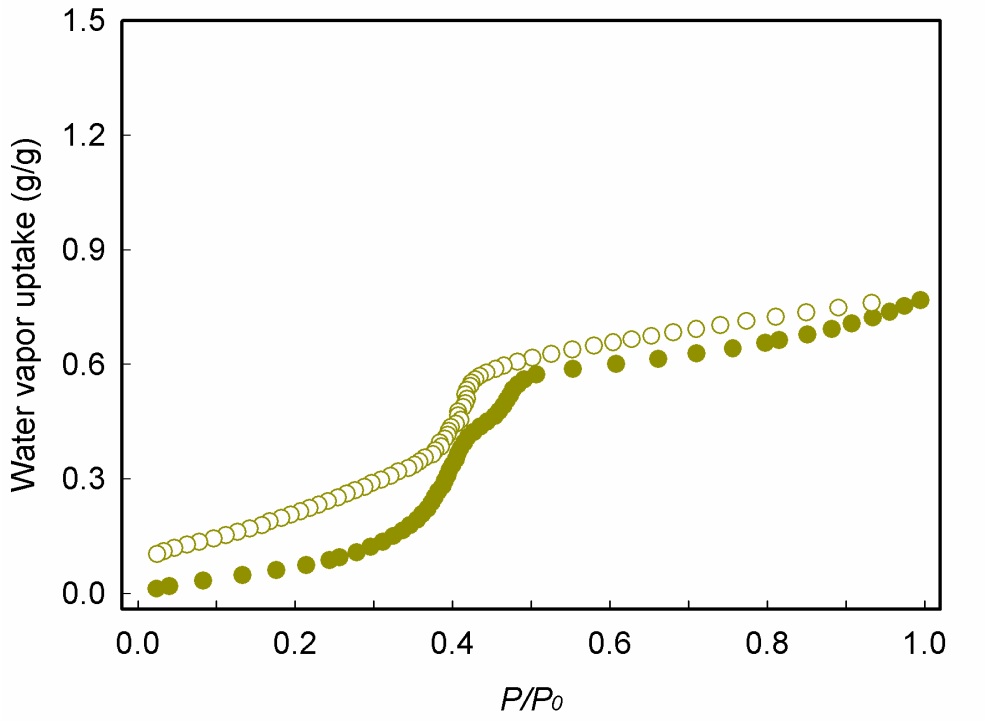

Fig. S5 Water vapor sorption isotherm of MIL-101-*p*Mal (**4**)

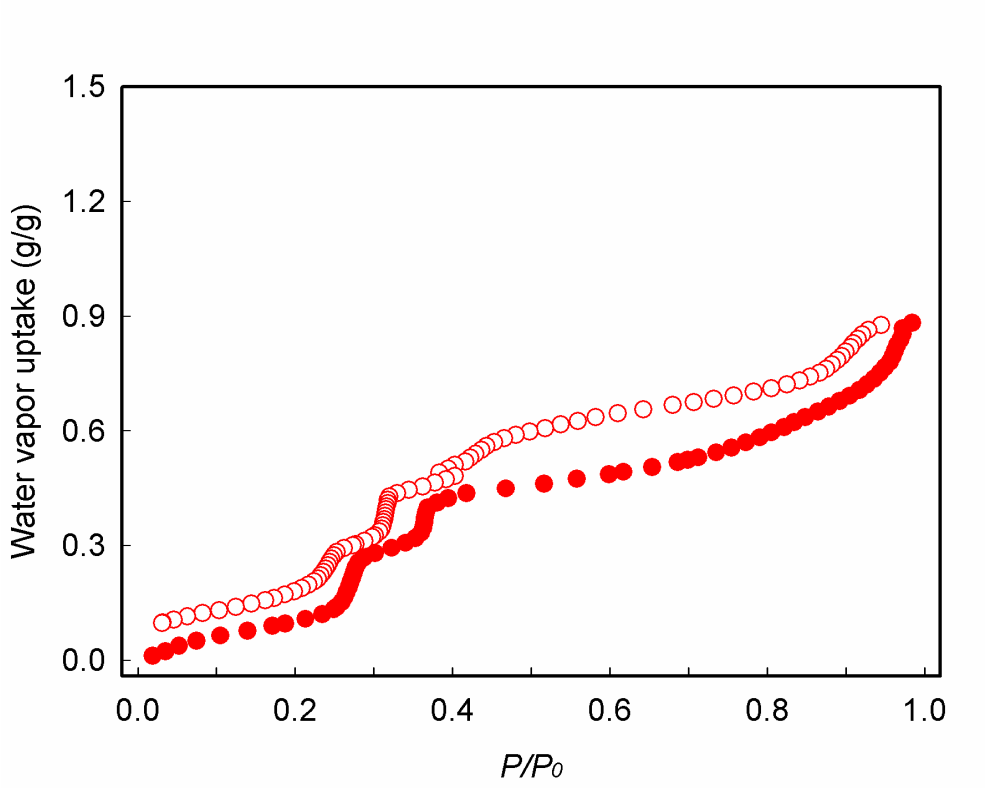

Fig. S6 Water vapor sorption isotherm of MIL-101-*p*3SO_3H (**5**).

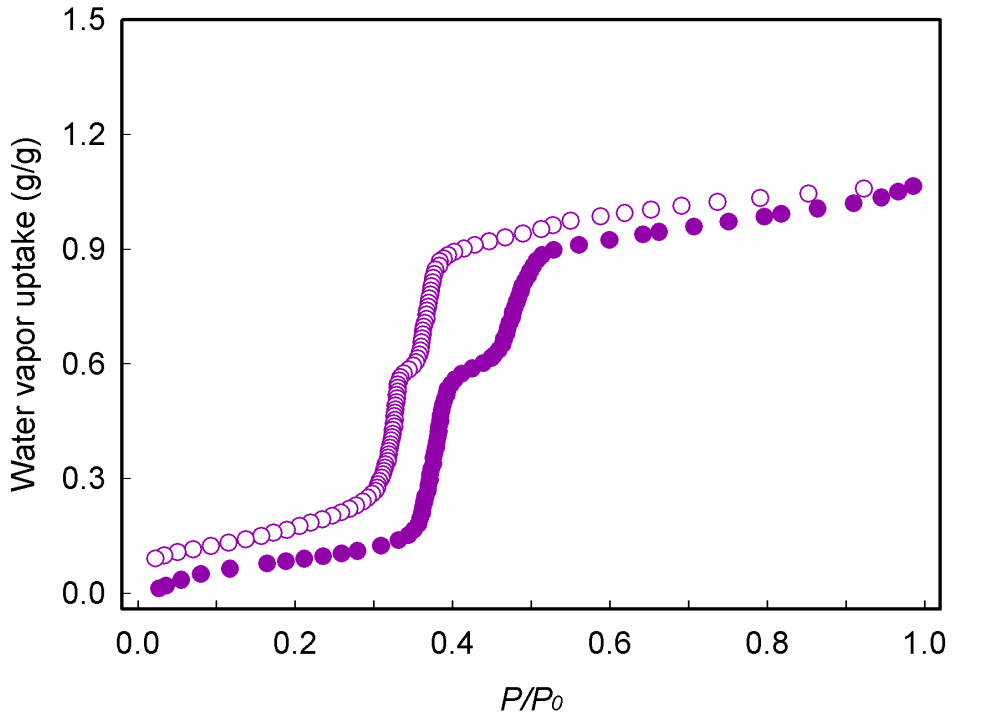

Fig. S7 Water vapor sorption isotherm of MIL-101-*p*COOH (**6a**).

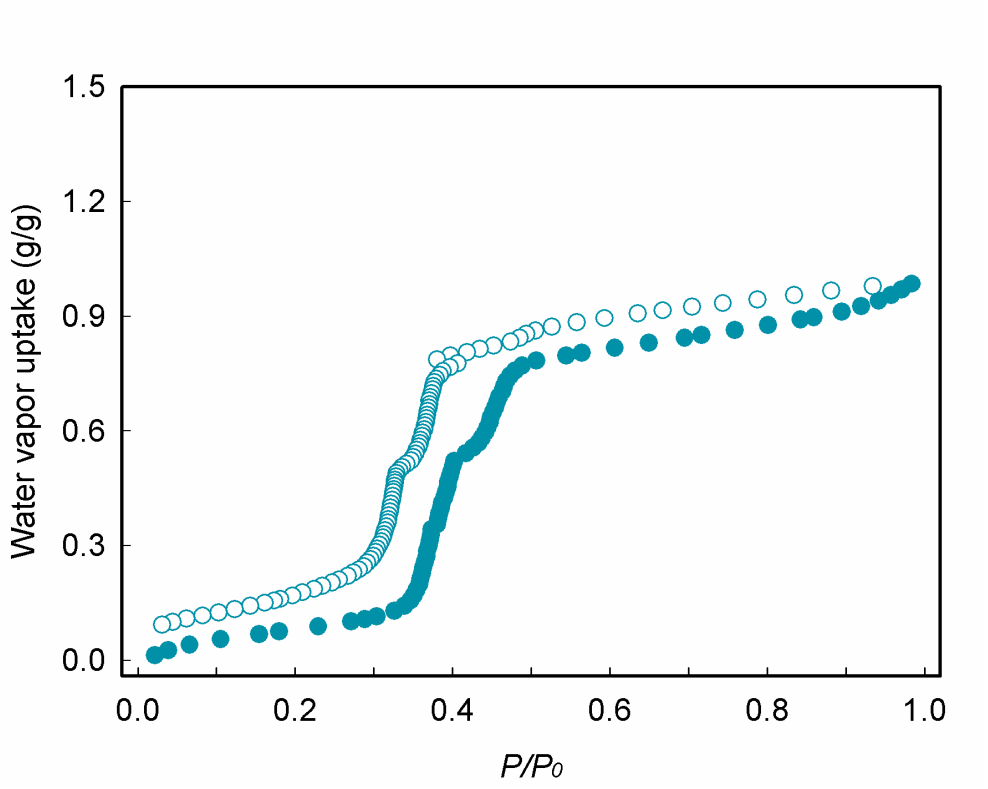

Fig. S8 Water vapor sorption isotherm of MIL-101-*p*COOH (**6b**).

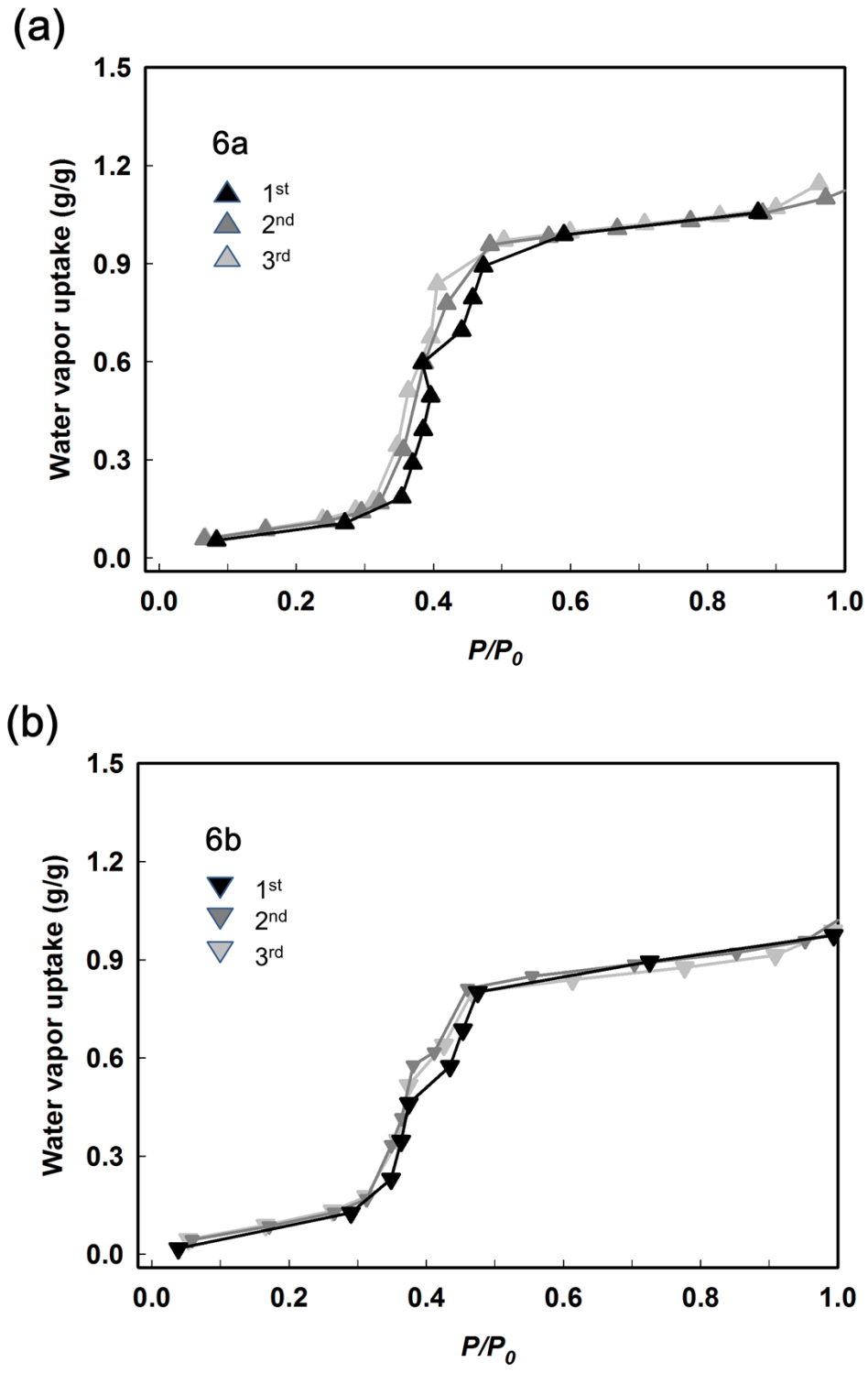

Fig. S9 Water vapor sorption isotherms of (a) MIL-101-*p*COOH (**6a**) and (b) MIL-101-*p*COOH (**6b**) obtained respectively for the repeated measurements using the sample samples.

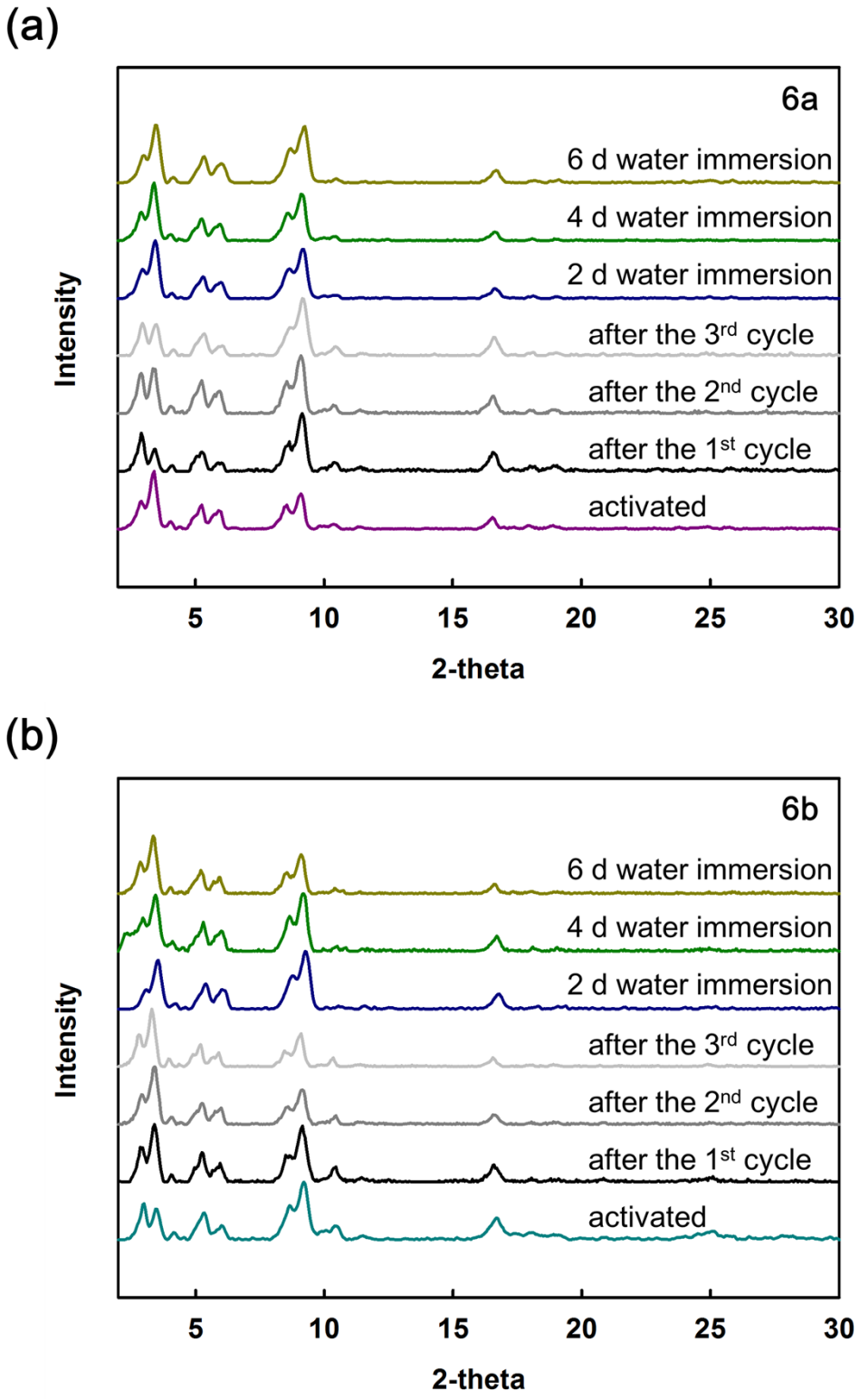

Fig. S10 PXRD patterns for (a) MIL-101-*p*COOH (**6a**) and (b) MIL-101-*p*COOH (**6b**) obtained respectively after the repeated water sorption measurements or water immersion up to six days.