Supporting information

Table S1. Synthesis conditions of solvothermal reactions to form UiO-66 solid, using $ZrCl_4$ (8.33mol) and H_2BDC (8.33 mmol) in presence of different equivalents of NH_4OH (4M) and HAC per Zr.

Sample	NH_4OH /Zr(eq.)	HAC/Zr (eq.)
UiO-66-AS	0	50
UiO-66(0.24, 50)	0.24	50
UiO-66(0.48, 50)	0.48	50
UiO-66(0.72, 50)	0.72	50
UiO-66(0.96, 50)	0.96	50
UiO-66(1.92, 50)	1.92	50
UiO-66(2.88, 50)	2.88	50
UiO-66(3.84, 50)	3.84	50
UiO-66(4.80, 50)	4.80	50
UiO-66(2.88, 0)	2.88	0
UiO-66(2.88, 12.5)	2.88	1.25
UiO-66(2.88, 25)	2.88	25
UiO-66(2.88, 62.5)	2.88	62.5
Zr-MOF-NH_4	0.18[1]	-
Zr-MOF-NH_4-1	0.18[2]	-
Zr-MOF-NH_4-2	0.35[2]	-
Zr-MOF-NH_4-3	0.53[2]	-

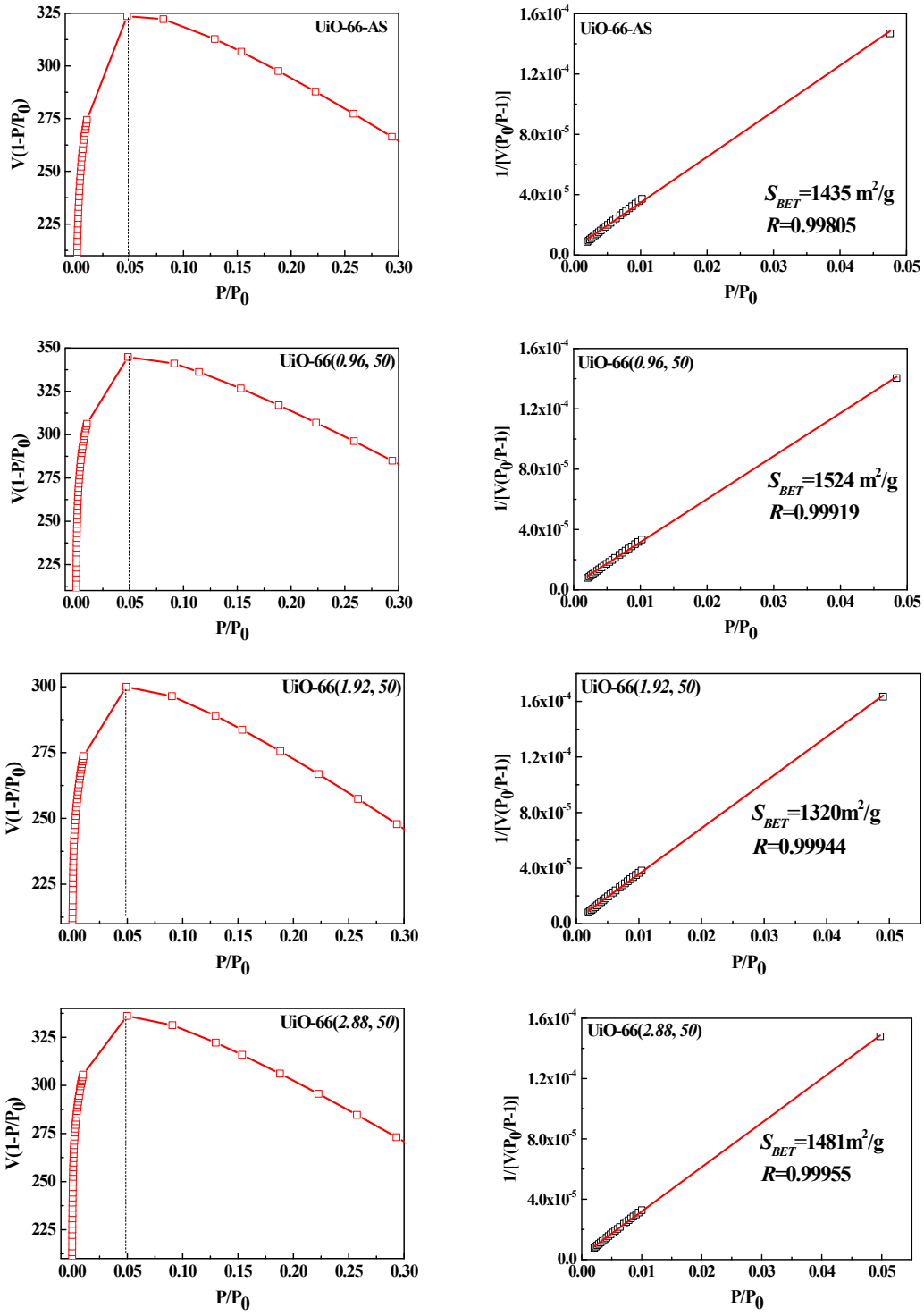
The mean particle size was determined by X-ray powder diffraction using the Debye–Scherrer equation, which estimates the particle size from the half width at mid-height of the most intense Bragg peak, namely (111) peaks for UiO-66 (Zr) (Fig. 2). It should be pointed out that the size of UiO-66-AS crystal is too large (>100 nm) to be calculated by Scherrer equation and the crystallite size of UiO-66-AS was figured out according to TEM pictures.

Table S2 Crystal size dermination of UiO-66 MOFs from the evaluation of XRD patterns using Scherrer's equation

Sample	2θ (°)	Radian	FWHM	Crystal size，nm
UiO-66-AS	-	-	-	300
UiO-66(0.96, 50)	7.27179	0.040399	0.23758	33.1
UiO-66(1.92, 50)	7.3158	0.040643	0.26992	29.1
UiO-66(2.88, 50)	7.29015	0.040501	0.30332	25.9
UiO-66(3.84, 50)	7.28122	0.040451	0.33314	23.6
UiO-66(4.80, 50)	7.28485	0.040471	0.40598	19.4
UiO-66(2.88, 0)	7.34913	0.128266516	2.12962	3.69
UiO-66(2.88, 12.5)	7.36384	0.128523254	1.75934	4.47
UiO-66(2.88, 25)	7.2957	0.127333986	0.59319	13.24

UiO-66(2.88, 62.5)	7.3371	0.12799	0.2715	28.9

Pressure range selected requires that not only the quantity of C constant must be positive , but the application of the BET equation should be limited to the pressure range where the term $V(P\text{-}P_0)$ or alternatively $V\,(1\text{-}P/P_0)$ continuously increases with P/P_0 (V is the adsorbed amount) according to criteria suggested by IUPAC recently[3]. As can be seen in Figure S1, it is clearly visible that all data points above a relative pressure of 0.05 have to be eliminated for application of the BET equation.



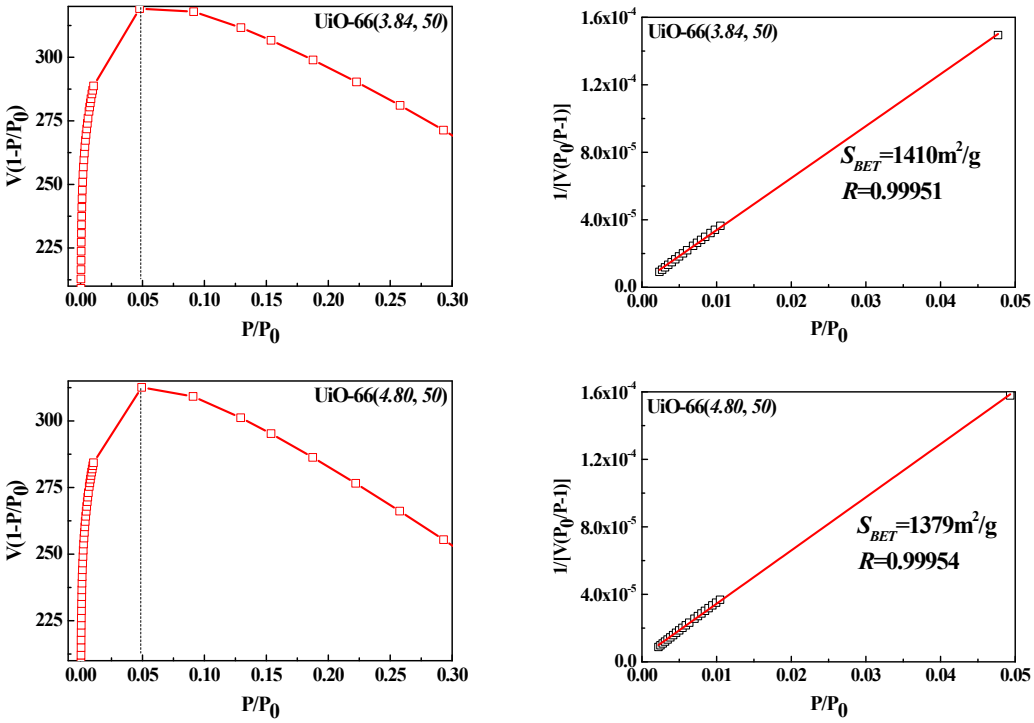


Figure. S1 Procedure of determination of the linear relative pressure range for BET analysis and BET plot for the selected linear data points.

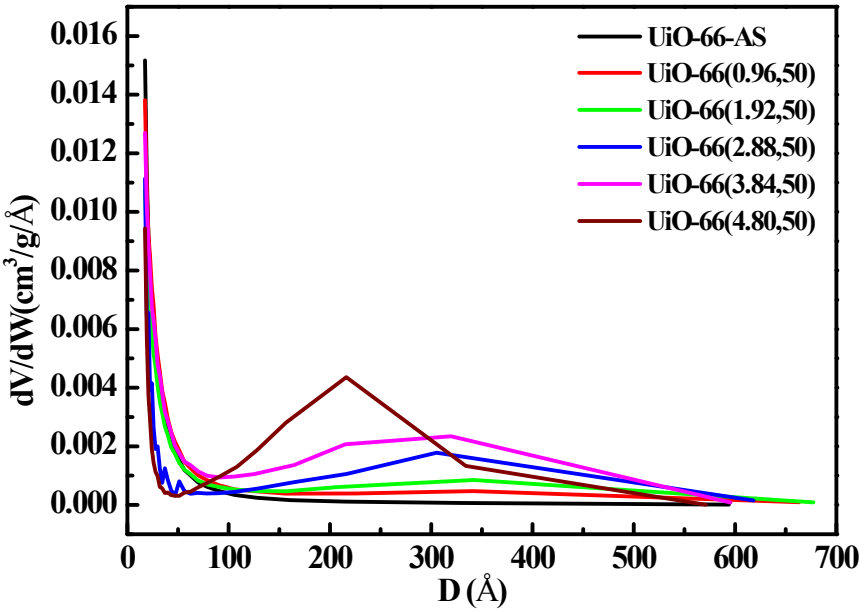


Figure S2 Pore size distributions (PSDs) calculated from desorption branch of N_2 isotherm by using BJH method.

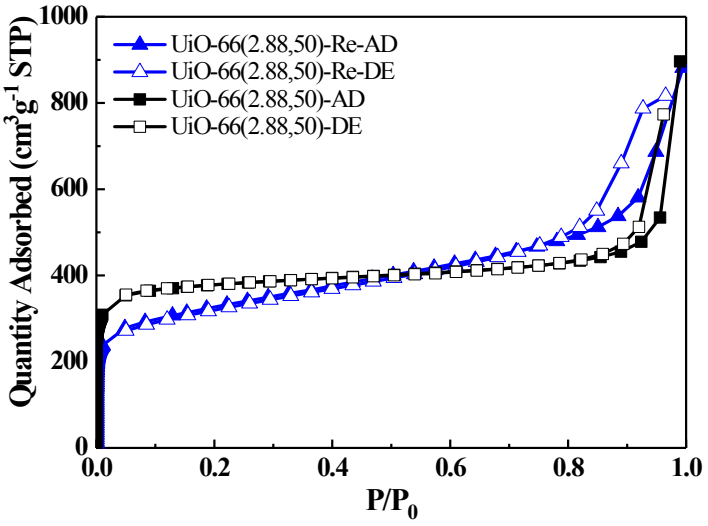


Figure S3 N_2 adsorption/desorption isotherms of UiO-66(2.88, 50) before and after MCH/nHEP sorption experiments at 77 K

Reference

[1] H.R. Abid, G.H. Pham, H.M. Ang, J. Colloid Interface Sci. **2012**, 366, 120-124.

[2] H.R. Abid, H.M. Ang, S. Wang, Nanoscale **2012**, 4, 3089-3094.

[3] J. Moellmer, E.B. Celer, R. Luebke, Microporous Mesoporous Mater. **2010**, 129, 345-353.