Supplementary information

Metal-Organic Frameworks (MOFs) as highly efficient agents for boron removal and boron isotopes separation

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Section S1. Research on boron isotopes separation with boron adsorbents

Table S1 Research on boron isotopes separation with boron adsorbents.

Adsorbents	**Temperature (°C)**	**pH**	**Boron concentration (mmol·L^{-1})**	**Isotopes separation factor, S**	**Refs**
Strongly basic anion exchange resin					
Amberlite CG-400I	R. T.	Not mention	100 [a]	1.016	[1]
Diaion PA-312	25	>12 [b]	10.4	1.019	[2]
Diaion SA-20A	25	12 [b]	106	1.011	[2]
Weakly basic anion exchange resin					
Diaion WA-21	5	10.5-11 [b]	10.4	1.023	[2]
Diaion WA-10	25	11-11.5 [b]	10.1	1.016	[2]
Diaion WA 30	25	11.5 [b]	9.99	1.017	[2]
Muromac 1×8	25	neutral	0.10	1.018	[3]
Muromac 1×8	25	neutral	0.10	1.012	[3]
Boron-selective resin					
CRB-02	25(50)	Not mention	100	1.018-1.022	[4]
N-Methyl-*D*-Glucamine Type Resin	Not mention	<7	100 [c]	1.027	[5]
Clay					
Kaolin	20	5	10.10	1.0023	[6]
Kaolin	25	5	9.51	1.0011	[7]
Other adsorbents					
$Mg(OH)_2$	25	10.5	45.9 [c]	1.022	[8]
Humic acids	25	5	3	1.027	[9]

[a] containing 8 wt. % purified glycerol.

[b] pH of the resin phase.

Section S2. Summary of boron adsorbents.

Table S2 Summary of boron adsorbents.

Adsorbents	Temperature (°C)	pH	Residual boron concentration (mmol·L^{-1})	Adsorption capacity (mmol·g^{-1})	Refs
Chelating resins					
Amberlite IRA-743	25	7.0	8.00	0.71	[10]
Pyrocatechol modified resin	25	9.0	2.00	0.42	[11]
poly(*N*-(4-vinylbenzyl)-*N*-methyl-*D*-glucamine) (P(VbNMDG))	25	-	1.850 ^{a}	98% ^{b}	[12]
Industrial waste					
Fly ash	25	10-11	1.00 ^{a}	94% ^{b}	[13]
Palm oil mill boiler bottom ash	25	8.0	1.20	0.0435	[14]
Calcined magnesite tailing	45	6.0	50.90	6.1	[15]
Natural materials					
Calcined Alunite	25	10.0	16.70	0.31	[16]
Calcium alginate gel	25	9-10	18.50 ^{a}	94	[17]
Waste sepiolite	20	10	55.50 ^{a}	16.52	[18]
New type inorganic sorbents					
MG modified SBA-15	25	7-12	0.93 ^{a}	45% ^{b}	[19]
MG modified MCM-41	25	6	9.25×10^{-4} ^{a}	0.8	[20]
Mg/Al layered double hydroxide	25	10	46.07 ^{a}	90% ^{b}	[21]
Si-MG	25	7	0.20	1.54	[22]
ZIF-8	25	-	500 ^{a}	17.67	This study

^{a} Initial boron concentrations (mmol·L^{-1}).

^{b} boron recovery efficiency.

Section S3. Characterization of ZIF-8

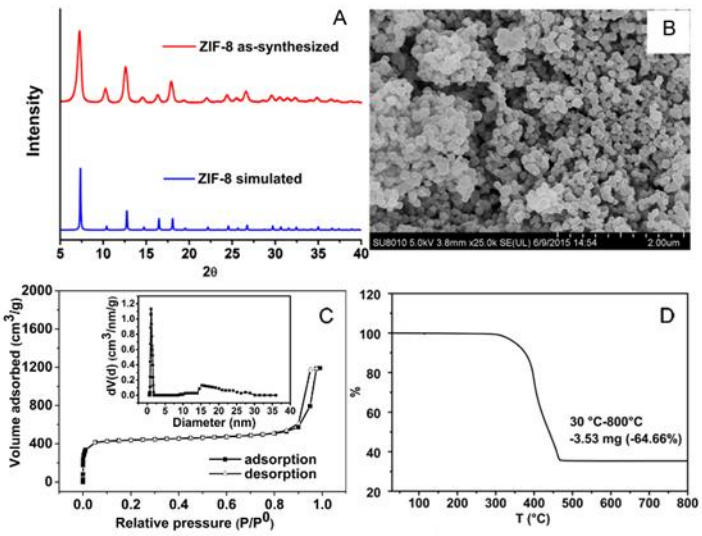

Fig. S1. Characterization of ZIF-8. a) XRD patterns; b) SEM image; c) N_2 adsorption/desorption isotherms and the pore size distribution (inset); d) TGA curve.

Section S4. Characterization of UiO-66

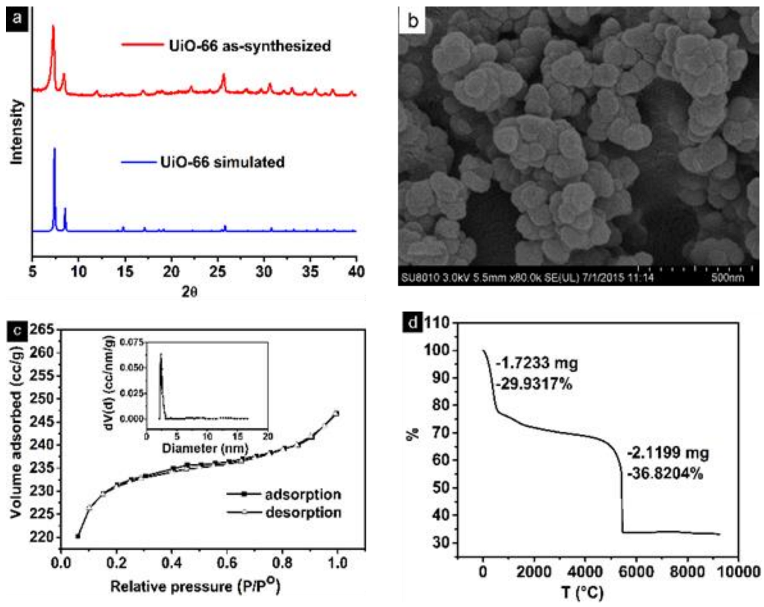

Fig. S2. Characterization of UiO-66. a) XRD patterns; b) SEM image; c) N_2 adsorption/desorption isotherms and the pore size distribution (inset); d) TGA curve.

Section S5. Characterization of MIL-100(Fe)

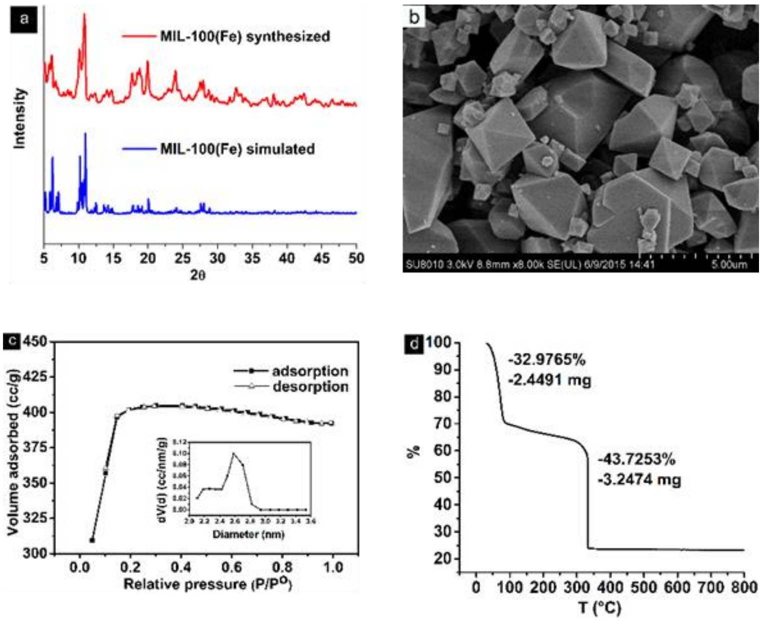

Fig. S3. Characterization of MIL-100(Fe). a) XRD patterns; b) SEM image; c) N_2 adsorption/desorption isotherms and the pore size distribution (inset); d) TGA curve.

Section S6. Characterization of MIL-101(Cr)

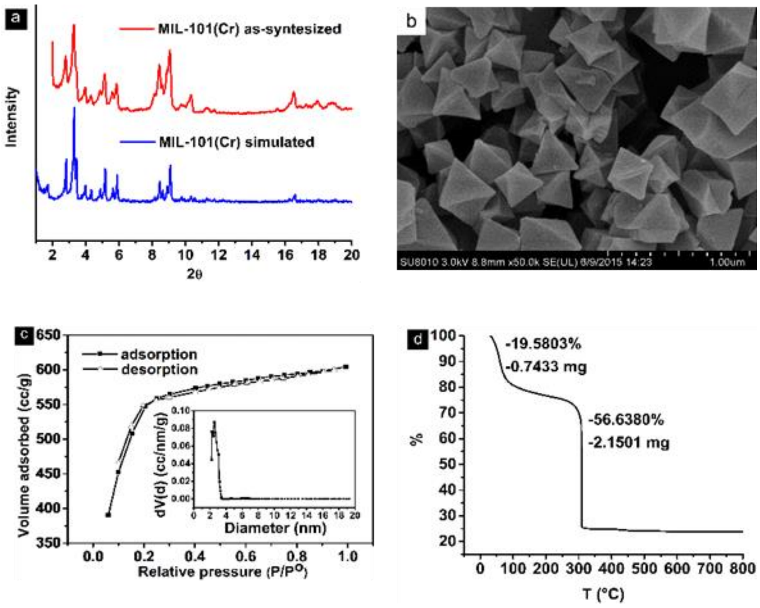

Fig. S4. Characterization of MIL-101(Cr). a) XRD patterns; b) SEM image; c) N_2 adsorption/desorption isotherms and the pore size distribution (inset); d) TGA curve.

Section S7. Characterization of MIL-100(Cr)

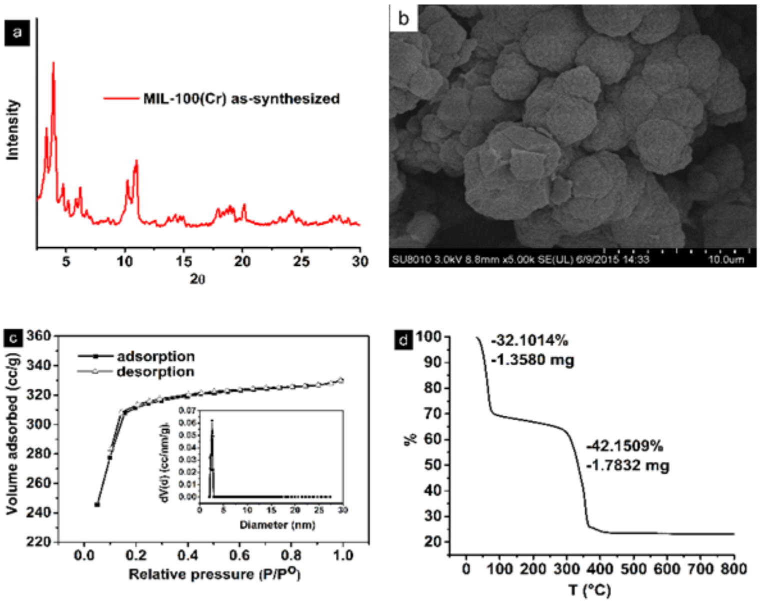

Fig. S5. Characterization of MIL-100(Cr). a) XRD patterns; b) SEM image; c) N_2 adsorption/desorption isotherms and the pore size distribution (inset); d) TGA curve.

Section S8. Characterization of MIL-53(Cr)

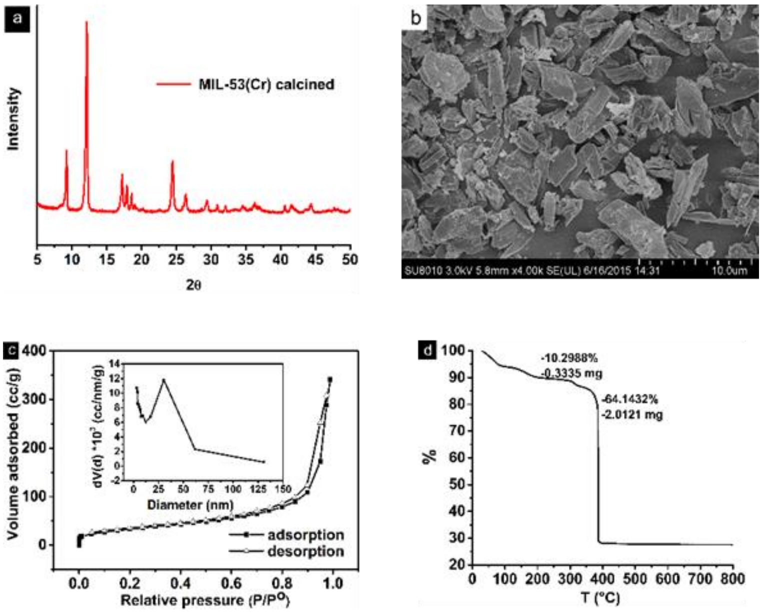

Fig. S6. Characterization of MIL-53(Cr). a) XRD patterns; b) SEM image; c) N_2 adsorption/desorption isotherms and the pore size distribution (inset); d) TGA curve.

Section S9. Characterization of MIL-96(Al)

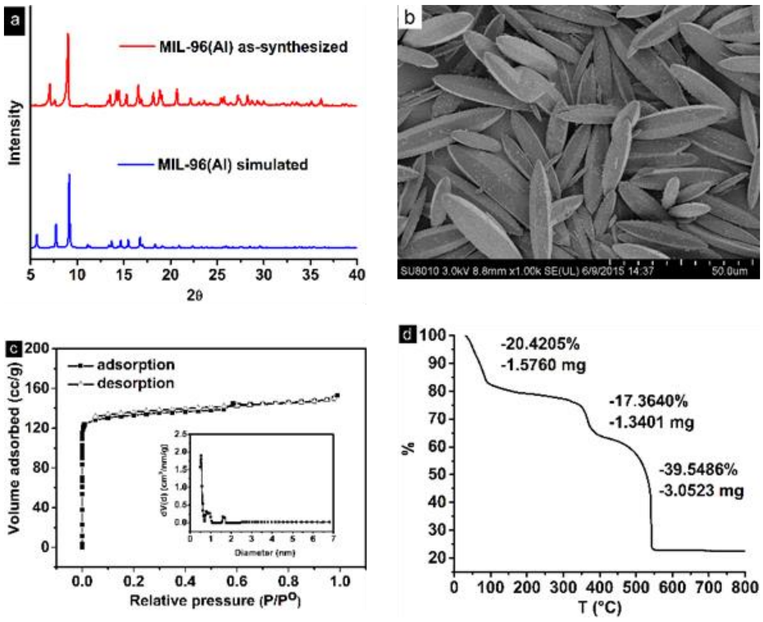

Fig. S7. Characterization of MIL-96(Al). a) XRD patterns; b) SEM image; c) N_2 adsorption/desorption isotherms and the pore size distribution (inset); d) TGA curve.

Section S10. Calculation of separation factor and adsorption capacity

The boron adsorption capacity Q ($mg \cdot g^{-1}$) can be calculated based on the following equation:

$$Q = \frac{(c_0 - c_1)M}{D} \times 1000 \tag{1}$$

where c_0 represents initial boron concentration, $mol \cdot L^{-1}$; c_1 represents residual boron concentration, $mol \cdot L^{-1}$; M means the molecular weight of boron, 10.81 $g \cdot mol^{-1}$; D means the dosage of adsorbents, 5 $g \cdot L^{-1}$.

The separation factor S can be calculated according to following equation:

$$\begin{aligned} S(^{10}B/^{11}B) &= \left[^{10}B/^{11}B\right]_{adsorbent} \Big/ \left[^{10}B/^{11}B\right]_{solution} \\ &= \left[\left(c_0 \cdot \frac{\alpha_0}{\alpha_0+1} - c_1 \cdot \frac{\alpha_1}{\alpha_1+1}\right) / \left(c_0 \cdot \frac{1}{\alpha_0+1} - c_1 \cdot \frac{1}{\alpha_1+1}\right)\right] \Big/ \alpha_1 \\ &= \frac{c_0\alpha_0(1+\alpha_1) - c_1\alpha_1(1+\alpha_0)}{c_0\alpha_1(1+\alpha_1) - c_1\alpha_1(1+\alpha_0)} \end{aligned} \tag{2}$$

$$S(^{11}\mathrm{B}/^{10}\mathrm{B}) = \frac{1}{S(^{10}\mathrm{B}/^{11}\mathrm{B})} \tag{3}$$

where α_0 represents initial $^{10}B/^{11}B$ abundance, 0.24779; α_1 represents $^{10}B/^{11}B$ abundance of the residual solution.

Section S11. Boron concentration and isotopic abundance of residual boron aqueous solutions

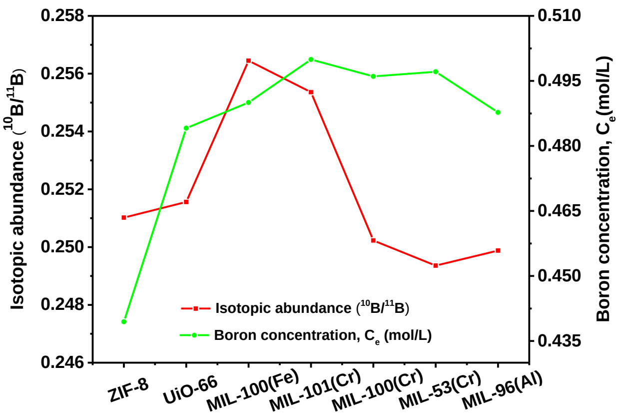

Fig. S8. boron concentration and isotopic abundance of residual boron aqueous solutions.

Section S12. Boron adsorption mechanism on ZIF-8

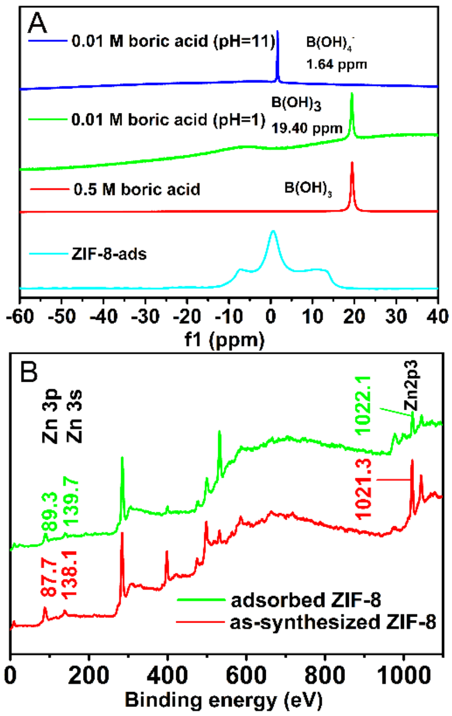

Fig. S9 (A) ^{11}B NMR of boric acid aqueous solutions and adsorbed ZIF-8; (B) XPS patterns of adsorbed and as-synthesized ZIF-8.

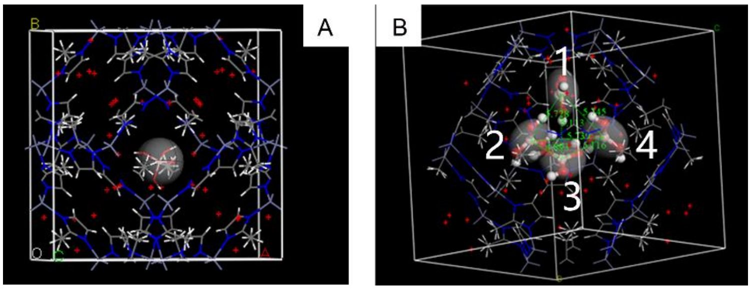

Fig. S10 (A) Simulation of boron adsorption in the style of $B(OH)_4^-$ on ZIF-8; (B) Simulation of boron adsorption in the style of $B(OH)_3$ on ZIF-8. (Task: locate, Method: metropolis, Quality: customized, Force field: Universal).

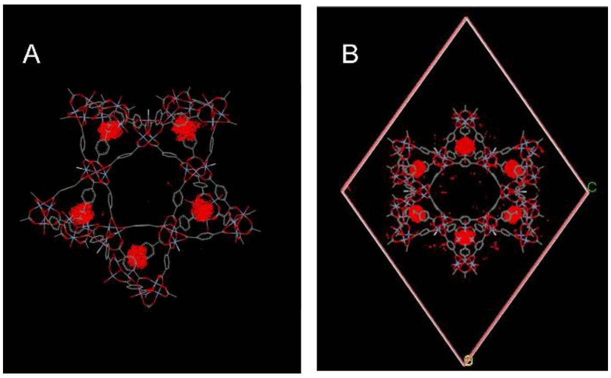

Fig. S11 Simulation of boron adsorption in the style of $B(OH)_3$ on MIL-101(Cr). The red in the cages represents the adsorbed boric acid molecules. (A) pentagonal window; (B) hexagonal window. (Task: locate, Method: metropolis, Quality: customized, Force field: Universal).

Section S13. References

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