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Supporting Information

"Solvent dependant supramolecular self-assembly of boron cage pillared metal-organic frameworks for selective gas separation"

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Table S1. Langmuir-Freundlich parameters fit for C_2H_2, CO_2 and C_2H_4 adsorption in BSF-4.

	Site A			Site B			correlation coefficient
	$q_{A,sat}$ (mol/kg)	b_A (kPa^{-1})	V_A	$Q_{B,sat}$ (mol/kg)	b_A (kPa^{-1})	V_B	(R^2)
C_2H_2 273K	1.410	1.748	0.985	3.439	0.038	0.607	0.99998
	1.629	1.600	1	1.764	0.017	1	0.99990
C_2H_2 298K	1.622	0.435	0.958	2.683	0.006	0.922	0.99999
	2.027	0.0066	1	1.578	0.452	1	0.99997
C_2H_2 313K	2.204	0.007	0.882	1.30	0.214	1.042	0.99993
	2.106	0.003	1	1.429	0.202	1	0.99993
CO_2 298K	2.506	0.0166	1	--	--	--	0.99998
C_2H_4 298K	1.656	0.079	0.972	1.018	4.75E-06	2.19	0.99996
	1.727	0.0684	1				0.9991

Table S2. Langmuir-Freundlich parameters fit for C_3H_8, C_2H_6 and CH_4 adsorption in BSF-5 at 298 K.

	Site A			Site B			correlation coefficient
	$q_{A,sat}$ (mol/kg)	b_A (kPa^{-1})	V_A	$Q_{B,sat}$ (mol/kg)	b_A (kPa^{-1})	V_B	(R^2)
C_3H_8	1.171	0.00756	1.002	0.5677	0.1216	1.8426	0.9991
C_2H_6	4.168	0.0189	0.4656	0.1206	0.022	1.991	0.9996
CH_4	0.435	0.0009	1.546	0.322	0.059	0.575	0.9999
	1.056	0.005	1	0.021	1.937	1	0.9999
	0.806	0.0086	1	--	--	--	0.998

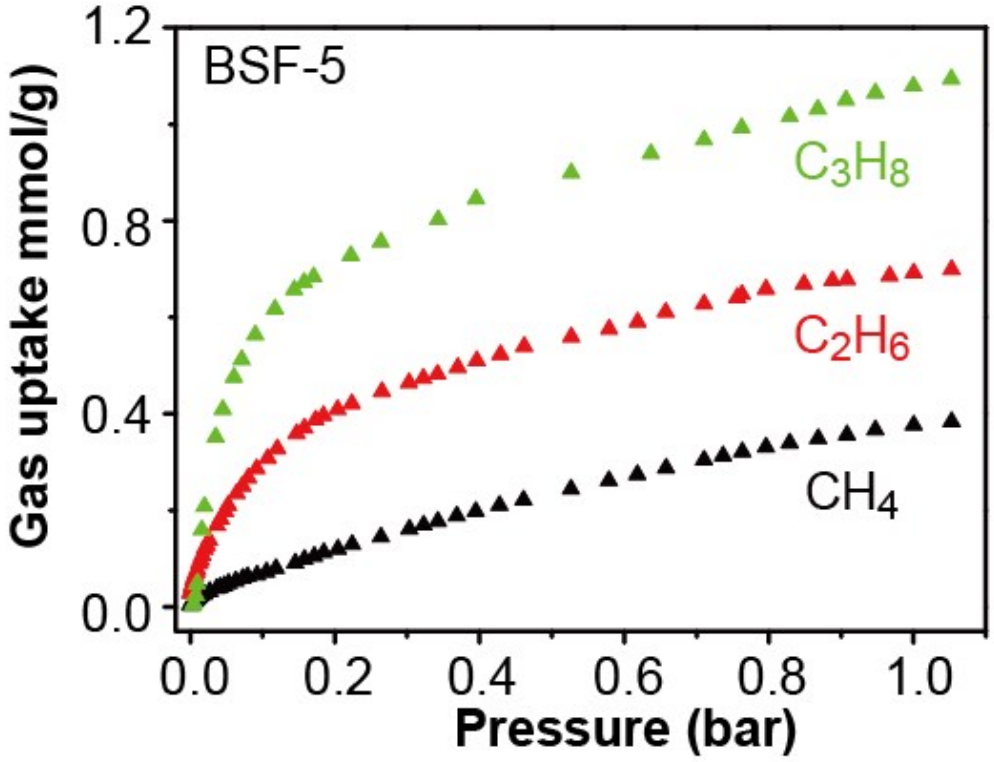

Fig. S1 C_3H_8, C_2H_6, CH_4 adsorption isotherms on activated BSF-5 at 298K.

Analysis: the C_3H_8, C_2H_6 and CH_4 uptakes at 298 K and 1 bar were 1.09, 0.70 and 0.38 mmol/g respectively. These values are all very low compared to those of BSF-1. However, it is understandable and consistent with the instability of BSF-5 that was supposed according to the N_2 adsorption experiment and PXRD patterns. The C_3H_8 capacity was further reduced to 0.9 mmol/g after the activated sample was exposed to air for a week. The calculated C_3H_8/CH_4 (1/1) and C_2H_6/CH_4 (1/1) IAST selectivity is 7.6 and 2.3.