Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Molecular Magnetism in Nanodomains of Isoreticular MIL-88(Fe)-MOFs

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Table 1: XPS survey analysis and elemental compositions and binding energies of each elements for all three MIL-88 analogues

Elemental transition peak	Energy (eV)	Chemical & oxidation states	% Weight (Experimental)	% Weight (Experimental)
		MIL-88B		
C 1s	283.42 & 286.23	C-C, C-O-C	41.41	41.54
O1s	530.19	Fe-O-C	32.73	32.28
Fe 2p **$2p_{3/2}$ & $2p_{1/2}$**	710.83, 715.53 723.78	Fe^{+2} & Fe^{+3}	24.77	24.14
		MIL-88C		
C1s	284.54 & 287.37	C-C, O-C=O	50.89	50.86
O1s	530.28	Fe-O-C	27.05	26.35
Fe 2p **$2p_{3/2}$ & $2p_{1/2}$**	710.83, 715.53, 723.78	Fe^{+2} & Fe^{+3}	20.17	19.71
		MIL-126		
C1s	284.54 & 287.37	C-C, O-C=O	50.89	50.86
O1s	530.28	Fe-O-C	27.05	26.35
Fe 2p **$2p_{3/2}$ & $2p_{1/2}$**	710.83, 715.53, 723.78	Fe^{+2} & Fe^{+3}	20.17	19.71

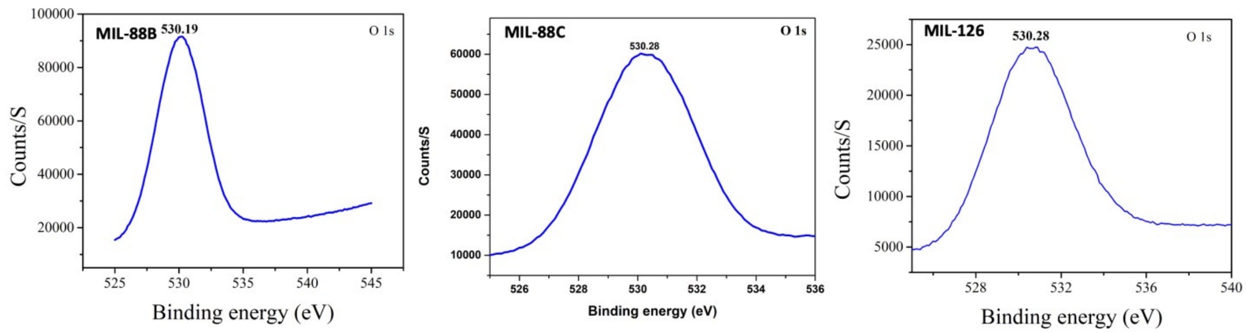

Figure S1: The binding energy O 1s spectra for all three analogues of MIL-88 analogues.

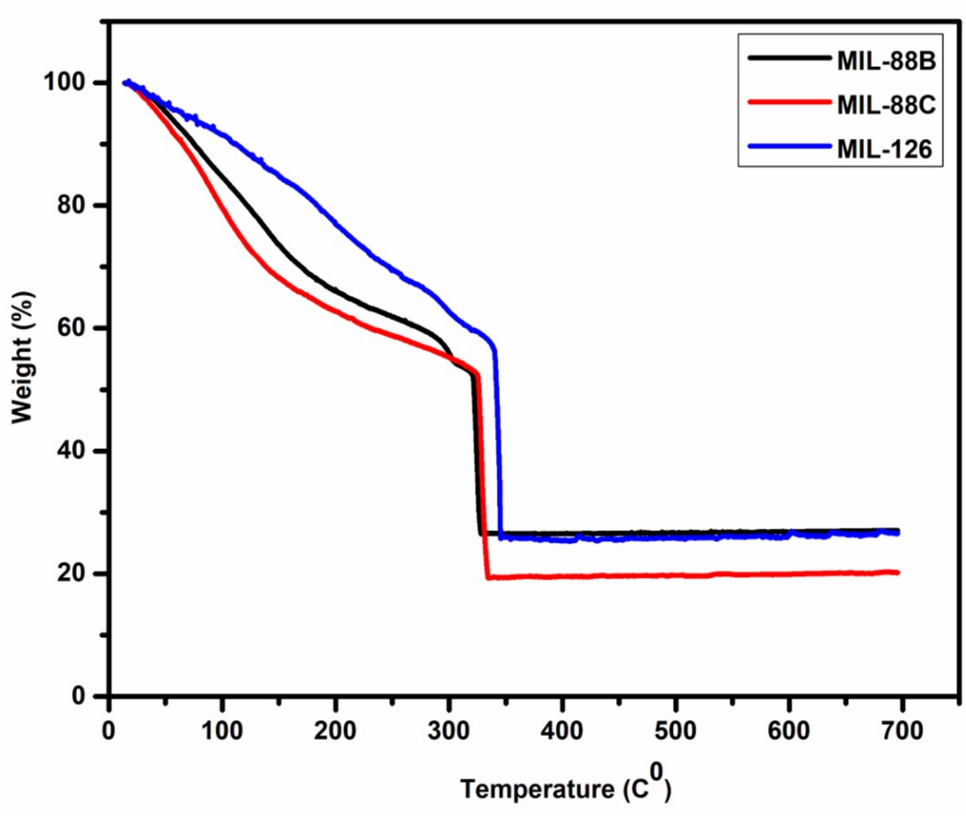

Figure S2: Thermal stabilities of all three analogues of MIL-88.

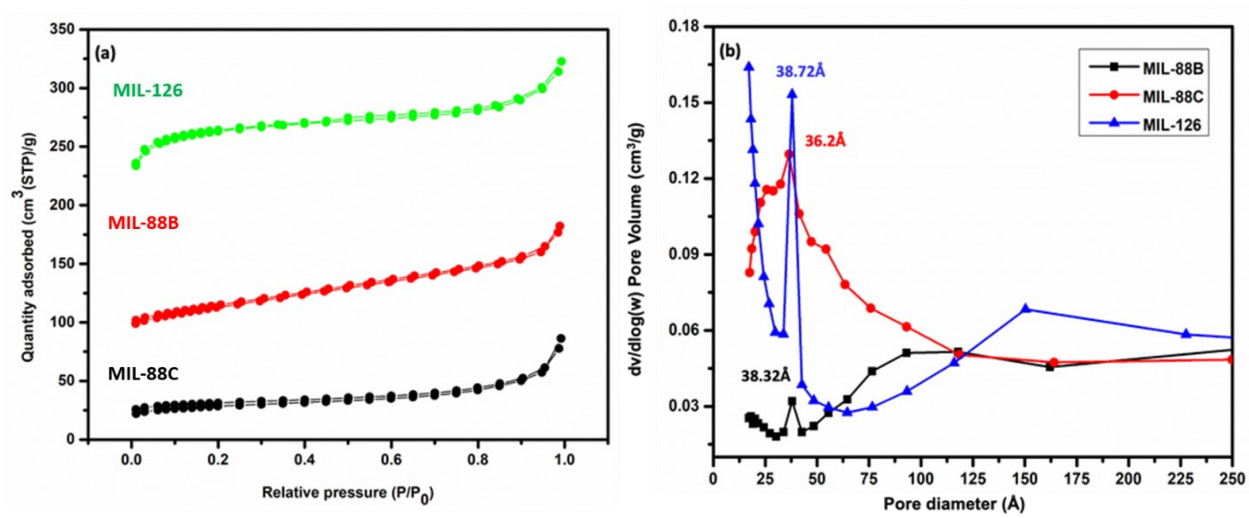

Figure S3: (a) The isotherms of MIL-88B, MIL-88C, and MIL-126; (b) The BJH pore distributions for MIL-88(Fe)-MOFs

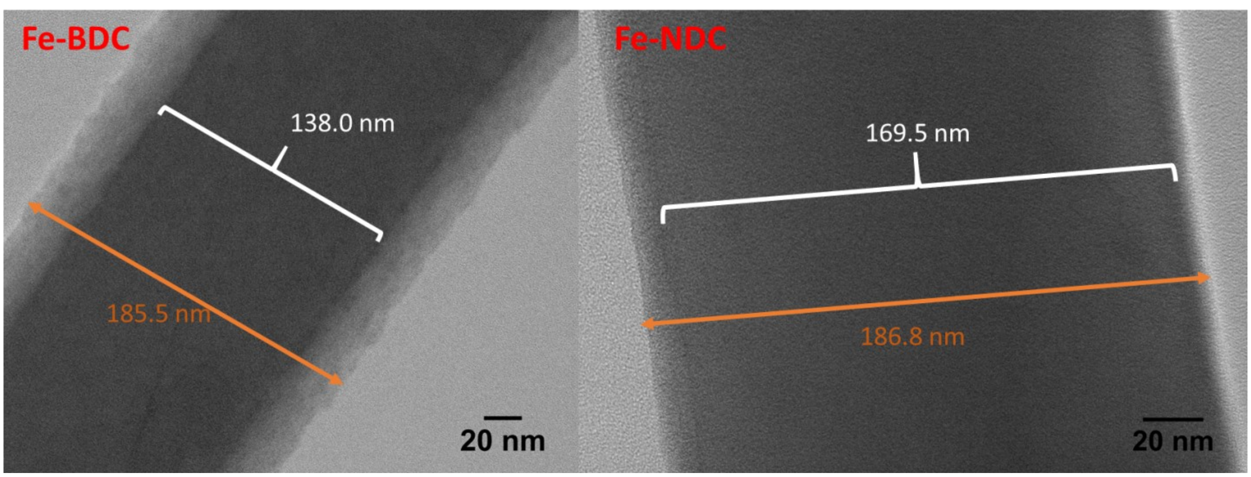

Figure S4. The thicknesses of the core and the shell are found to be ~138 nm and ~47.5 nm for MIL-88B and 169.8 nm and 17.3 nm for MIL-88C, respectively (Figure S4).

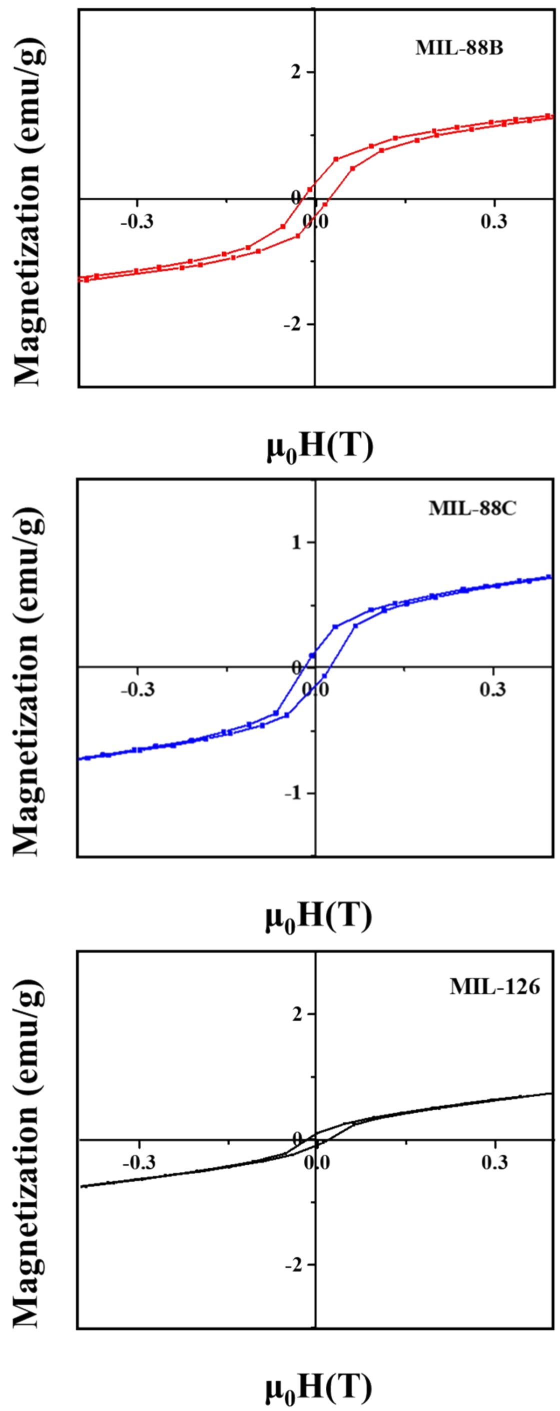

Figure S5: M-H loops for three MIL-88(Fe) MOFs at 10 K.