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

Supporting Information

DFT Insights into the Adsorption of NH_3-SCR Related Small Gases in Mn-MOF-74

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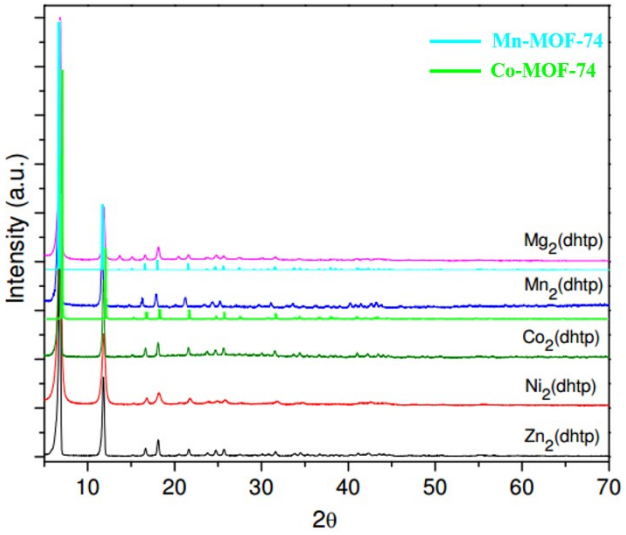

Fig. S1 Comparison between experimental and calculated PXRD patterns of Mn-MOF-74 and Co-MOF-74

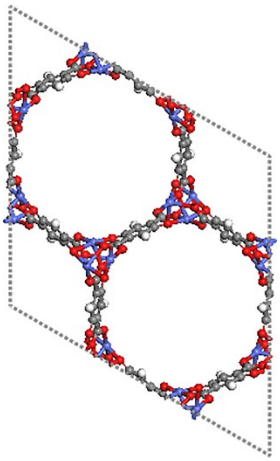

Fig. S2 DFT optimized Co-MOF-74 structure

Table S1. Comparison of lattice parameters of Co-MOF-74 between experimental results and DFT optimization

Co-MOF-74 lattice constant（Å）	Experimental data[1]	Experimental data[2]	Our Calculated data
a	26.132	25.948	25.877
b	26.132	25.948	25.877
c	6.722	6.838	6.866

References

[1] Ng. W. Wong, J. A. Kaduk and H. Wu, Synchrotron X-ray studies of metal-organic framework M2 (2, 5-dihydroxyterephthalate), M=(Mn, Co, Ni, Zn)(MOF-74), *Powder Diffr*., 2012, **27**, 256-262.

[2] W. Zhou, H. Wu and T. Yildirim, Enhanced H_2 adsorption in isostructural metal-organic frameworks with open metal sites: strong dependence of the binding strength on metal ions, *J. Am.Chem. Soc*., 2008, **130**(130), 15268-15269.

Table S2. Optimized geometries of adsorbed NH_3-SCR related small gases in Mn-MOF-74

Molecule	Bond name	Bond length(Å)
NH_3	Mn-N	2.059
	N-H1*	1.032
	N-H2*	1028
	N-H3*	1.030
NO	Mn-N	2.011
	N-O*	1.207
O_2	Mn-O	2.053
	O-O*	1.319
NO_2	Mn-N	2.064
	N-O1*	1.364
	N-O2*	1.374
H_2O	Mn-O	2.200
	O-H1*	0.994
	O-H2*	0.995
$SO_{2(1)}$[a]	Mn-O	2.014
	S-O1*	1.618
	S-O2*	1.553
$SO_{2(2)}$[b]	Mn-S	2.547
	S-O1*	1.559
	S-O2*	1.556

* means the intramolecule bond lengths of the adsorbed gas molecules;

[a]$SO_{2(1)}$ refers to the configuration when SO_2 adsorbs in the Mn-MOF-74 in the form of O end adsorption, while [a]$SO_{2(2)}$ is the case of S end adsorption.