Electronic Supplementary Material (ESI) for CrystEngComm

The Effect of Earth Metal ion on the Property of Peptide - based Metal-Organic Frameworks

Wu-lin Chen,[a] Wen-Xian Chen, [a] Gui-lin Zhuang,[a]* Jun Zheng,[b] Li Tan,[a] Xing Zhong,[a] Jian-guo Wang*[a]

[a]*Institute of Industrial Catalysis, College of Chemical Engineering and Materials Science, Zhejiang University of Technology, Hangzhou, People's Republic of China, 310032.*

Fax: (+86)571-88871037 Tel: (+86)571-88871037

E-mail: glzhuang@zjut.edu.cn, jgw@zjut.edu.cn

[b] Center of Modern Experimental Technology, Anhui University, Hefei, People's Republic of China,230039.

1. XRD pattern of compounds 1-4

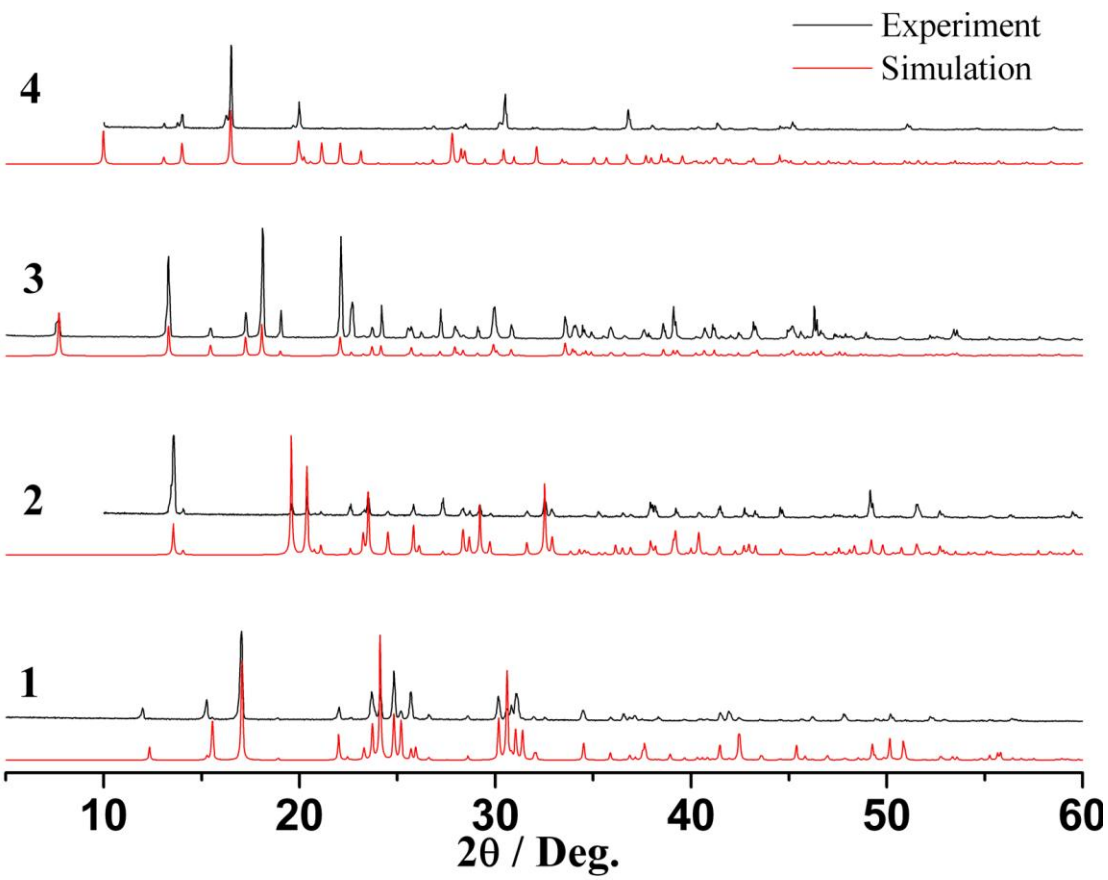

Fig. S1 Experimental and theoretical XRD pattern of compounds 1-4.

2. Theoretical UV-vis adsorption spectra of 4

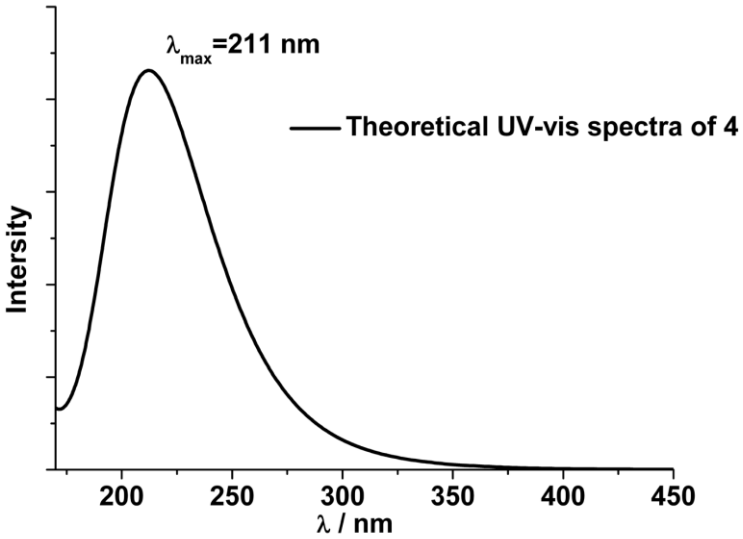

Fig. S2 UV-vis adsorption spectra of 4 under DFT simulation.

3. Thermogravimetric curves of 1-4

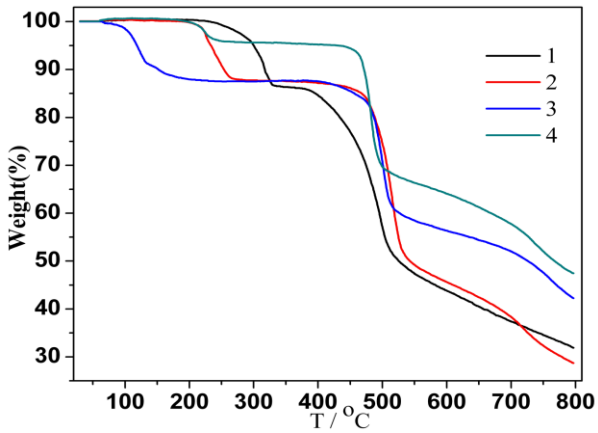

Fig. S3 TG curve of 1-4 at the range from room temperature to 800 °C.

4. Crystal data, bond lengths and angle for compounds 1-4

Table S1 Crystal data and details of data collection and refinement for compounds 1–4

Compounds	**1**	**2**	**3**	**4**
Formula	$C_8H_{12}N_2O_8Mg$	$C_8H_{12}N_2O_8Ca$	$C_8H_{14}N_2O_9Sr$	$C_8H_{10}N_2O_7Ba$
Mr	288.51	304.28	369.83	383.52
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P*2(1)/c	*P*2(1)/n	*C*2/c	*C*2/c
a/Å	7.5673(5)	7.5941(4)	23.6213(16)	4.6423(2)
b/Å	9.3773(5)	5.6569(3)	6.9431(5)	13.5308(6)
c/Å	7.7862(5)	13.1056(6)	8.0865(4)	17.7254(9)
α/deg	90.00	90.00	90.00	90.00
β/deg	108.734(7)	95.284(4)	104.072(9)	93.474(4)
γ/deg	90.00	90.00	90.00	90.00
V/Å^3	523.25(5)	560.61(5)	1286.43(14)	1111.36(9)

Z	2	2	4	4
*D*c/g cm^{-3}	1.831	1.803	1.910	2.292
μ/mm-1	0.215	0.602	4.239	3.605
Data/params	1021/96	1100/96	1258/104	1093/87
θ /deg	3.51-25.99	3.12-25.99	3.88-26.00	3.22-25.99
Obs reflns	927	990	1200	1088
Goof on F^2	1.192	1.129	1.049	1.214
$R1[I>2\sigma(I)]$[a]	0.0368	0.0257	0.0196	0.0159
$wR2$(All data)[b]	0.1116	0.0669	0.0501	0.0400

[a] $R_1 = \sum||FO| - |FC||/\sum|FO|$ [b] $wR_2 = \{\sum[w(FO2 - FC2)2]/\sum[w(FO2)2]\}1/2$

Table S2 Bond lengths and angle of compounds **1**-**4**

Compound 1			
Mg(1)-O(1W)#1	2.0336(15)	Mg(1)-O(1W)	2.0336(15)
Mg(1)-O(3)	2.0738(14)	Mg(1)-O(3)#1	2.0738(14)
Mg(1)-O(2)#2	2.1097(14)	Mg(1)-O(2)#3	2.1097(14)
O(1W)#1-Mg(1)-O(1W)	180.00(9)	O(1W)#1-Mg(1)-O(3)	92.80(6)
O(1W)-Mg(1)-O(3)	87.20(6)	O(1W)#1-Mg(1)-O(3)#1	87.20(6)
O(1W)-Mg(1)-O(3)#1	92.80(6)	O(3)-Mg(1)-O(3)#1	180.0
O(1W)#1-Mg(1)-O(2)#2	90.13(6)	O(1W)-Mg(1)-O(2)#2	89.87(6)
O(3)-Mg(1)-O(2)#2	87.34(6)	O(3)#1-Mg(1)-O(2)#2	92.66(6)
O(1W)#1-Mg(1)-O(2)#3	89.87(6)	O(1W)-Mg(1)-O(2)#3	90.13(6)
O(3)-Mg(1)-O(2)#3	92.66(6)	O(3)#1-Mg(1)-O(2)#3	87.34(6)
Compound 2			
Ca(1)-O(1W)	2.3273(14)	Ca(1)-O(1W)#1	2.3273(14)
Ca(1)-O(1)#2	2.3300(11)	Ca(1)-O(1)#3	2.3300(11)
Ca(1)-O(3)	2.3373(12)	Ca(1)-O(3)#1	2.3373(12)
O(1W)-Ca(1)-O(1W)#1	180.0	O(1W)-Ca(1)-O(1)#2	90.36(5)
O(1W)#1-Ca(1)-O(1)#2	89.64(5)	O(1W)-Ca(1)-O(1)#3	89.64(5)
O(1W)#1-Ca(1)-O(1)#3	90.36(5)	O(1)#2-Ca(1)-O(1)#3	180.0
O(1W)-Ca(1)-O(3)	91.81(5)	O(1W)#1-Ca(1)-O(3)	88.19(5)
O(1)#2-Ca(1)-O(3)	92.35(4)	O(1)#3-Ca(1)-O(3)	87.65(4)
O(1W)-Ca(1)-O(3)#1	88.19(5)	O(1W)#1-Ca(1)-O(3)#1	91.81(5)

O(1)#2-Ca(1)-O(3)#1	87.65(4)	O(1)#3-Ca(1)-O(3)#1	92.35(4)
O(3)-Ca(1)-O(3)#1	180.0		

Compound 3

Sr(1)-O(1)	2.579(8)	Sr(1)-O(6)#1	2.581(7)
Sr(1)-O(3W)	2.587(7)	Sr(1)-O(2W)	2.593(7)
Sr(1)-O(1W)	2.595(2)	Sr(1)-O(1)#2	2.729(8)
Sr(1)-O(6)#3	2.751(8)	Sr(1)-O(5)#3	2.810(9)
Sr(1)-O(2)#2	2.824(8)	Sr(1)-H(2WB)	2.65(11)
O(1)-Sr(1)-O(6)#1	166.79(6)	O(1)-Sr(1)-O(3W)	101.7(3)
O(6)#1-Sr(1)-O(3W)	73.1(2)	O(1)-Sr(1)-O(2W)	72.8(3)
O(6)#1-Sr(1)-O(2W)	101.7(3)	O(3W)-Sr(1)-O(2W)	133.67(9)
O(1)-Sr(1)-O(1W)	84.4(4)	O(6)#1-Sr(1)-O(1W)	82.4(4)
O(3W)-Sr(1)-O(1W)	66.6(3)	O(2W)-Sr(1)-O(1W)	67.1(3)
O(1)-Sr(1)-O(1)#2	120.9(3)	O(6)#1-Sr(1)-O(1)#2	69.7(2)
O(3W)-Sr(1)-O(1)#2	71.6(3)	O(2W)-Sr(1)-O(1)#2	151.2(3)
O(1W)-Sr(1)-O(1)#2	134.9(3)	O(1)-Sr(1)-O(6)#3	69.35(19)
O(6)#1-Sr(1)-O(6)#3	121.1(2)	O(3W)-Sr(1)-O(6)#3	150.6(3)
O(2W)-Sr(1)-O(6)#3	72.1(2)	O(1W)-Sr(1)-O(6)#3	136.5(3)
O(1)#2-Sr(1)-O(6)#3	88.65(5)	O(1)-Sr(1)-O(5)#3	112.1(3)
O(6)#1-Sr(1)-O(5)#3	76.1(3)	O(3W)-Sr(1)-O(5)#3	144.3(3)
O(2W)-Sr(1)-O(5)#3	70.1(3)	O(1W)-Sr(1)-O(5)#3	126.3(3)
O(1)#2-Sr(1)-O(5)#3	81.2(3)	O(6)#3-Sr(1)-O(5)#3	46.0(3)
O(1)-Sr(1)-O(2)#2	74.3(3)	O(6)#1-Sr(1)-O(2)#2	113.8(2)
O(3W)-Sr(1)-O(2)#2	69.5(3)	O(2W)-Sr(1)-O(2)#2	143.1(3)
O(1W)-Sr(1)-O(2)#2	125.3(3)	O(1)#2-Sr(1)-O(2)#2	47.7(2)
O(6)#3-Sr(1)-O(2)#2	81.1(3)	O(5)#3-Sr(1)-O(2)#2	108.35(7)
O(1)-Sr(1)-H(2WB)	85.9(19)	O(6)#1-Sr(1)-H(2WB)	92(2)
O(3W)-Sr(1)-H(2WB)	146(2)	O(2W)-Sr(1)-H(2WB)	19.0(7)
O(1W)-Sr(1)-H(2WB)	81.5(18)	O(1)#2-Sr(1)-H(2WB)	132.3(8)
O(6)#3-Sr(1)-H(2WB)	63(2)	O(5)#3-Sr(1)-H(2WB)	51.3(9)

O(2)#2-Sr(1)-H(2WB)	143(3)	C(8)#3-Sr(1)-H(2WB)	50.2(18)
C(1)#2-Sr(1)-H(2WB)	148.3(17)	Sr(1)#2-Sr(1)-H(2WB)	116.3(14)

Compound 4

Ba(1)-O(3)#1	2.779(2)	Ba(1)-O(3)	2.779(2)
Ba(1)-O(1)#2	2.8059(19)	Ba(1)-O(1)#3	2.8059(19)
Ba(1)-O(2)#4	2.852(2)	Ba(1)-O(2)#5	2.852(2)
Ba(1)-O(1)#4	2.942(2)	Ba(1)-O(1)#5	2.942(2)
Ba(1)-O(1W)	3.118(2)	Ba(1)-O(1W)#6	3.118(2)
O(3)#1-Ba(1)-O(3)	119.42(10)	O(3)#1-Ba(1)-O(1)#2	71.47(6)
O(3)-Ba(1)-O(1)#2	127.18(6)	O(3)#1-Ba(1)-O(1)#3	127.18(6)
O(3)-Ba(1)-O(1)#3	71.47(6)	O(1)#2-Ba(1)-O(1)#3	147.00(8)
O(3)#1-Ba(1)-O(2)#4	148.88(7)	O(3)-Ba(1)-O(2)#4	87.79(7)
O(1)#2-Ba(1)-O(2)#4	80.14(6)	O(1)#3-Ba(1)-O(2)#4	73.19(6)
O(3)#1-Ba(1)-O(2)#5	87.79(7)	O(3)-Ba(1)-O(2)#5	148.88(7)
O(1)#2-Ba(1)-O(2)#5	73.19(6)	O(1)#3-Ba(1)-O(2)#5	80.14(6)
O(2)#4-Ba(1)-O(2)#5	71.70(9)	O(3)#1-Ba(1)-O(1)#4	125.05(6)
O(3)-Ba(1)-O(1)#4	72.49(6)	O(1)#2-Ba(1)-O(1)#4	62.73(7)
O(1)#3-Ba(1)-O(1)#4	107.71(6)	O(2)#4-Ba(1)-O(1)#4	45.12(5)
O(2)#5-Ba(1)-O(1)#4	105.46(6)	O(3)#1-Ba(1)-O(1)#5	72.49(6)
O(3)-Ba(1)-O(1)#5	125.05(6)	O(1)#2-Ba(1)-O(1)#5	107.71(6)
O(1)#3-Ba(1)-O(1)#5	62.73(7)	O(2)#4-Ba(1)-O(1)#5	105.46(6)
O(2)#5-Ba(1)-O(1)#5	45.12(5)	O(1)#4-Ba(1)-O(1)#5	148.56(7)
O(3)#1-Ba(1)-O(1W)	70.39(5)	O(3)-Ba(1)-O(1W)	70.26(5)
O(1)#2-Ba(1)-O(1W)	141.55(5)	O(1)#3-Ba(1)-O(1W)	66.18(5)
O(2)#4-Ba(1)-O(1W)	138.07(5)	O(2)#5-Ba(1)-O(1W)	109.78(5)
O(1)#4-Ba(1)-O(1W)	142.15(5)	O(1)#5-Ba(1)-O(1W)	64.67(5)
O(3)#1-Ba(1)-O(1W)#6	70.26(5)	O(3)-Ba(1)-O(1W)#6	70.39(5)
O(1)#2-Ba(1)-O(1W)#6	66.18(5)	O(1)#3-Ba(1)-O(1W)#6	141.55(5)
O(2)#4-Ba(1)-O(1W)#6	109.78(5)	O(2)#5-Ba(1)-O(1W)#6	138.07(5)
O(1)#4-Ba(1)-O(1W)#6	64.67(5)	O(1)#5-Ba(1)-O(1W)#6	142.15(5)

O(1W)-Ba(1)-O(1W)#6	96.24(9)

Compound **1**: #1 -x+2, -y+2, -z; #2 -x+2, y-1/2, -z+1/2; #3 x, -y+5/2, z-1/2.
Compound **2**: #1 -x+1, -y, -z+2; #2 -x+1/2, y-1/2, -z+3/2; #3 x+1/2, -y+1/2, z+1/2.
Compound **3**: #1 x+1/2, -y+1/2, z-1/2; #2 x, -y, z-1/2; #3 x+1/2, y-1/2, z.
Compound **4**: #1 -x, y, -z+1/2; #2 -x+1/2, y+1/2, -z+1/2; #3 x-1/2, y+1/2, z; #4 x+1/2, y+1/2, z; #5 -x-1/2, y+1/2, -z+1/2; #6 x+1, y, z.

Table S3 Hydrogen-bond geometry (Å , °) of compounds **3**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*··· O6 ^{i}	0.85	2.42	3.071(11)	134
O1*W*—H1*WB*··· O1 ^{ii}	0.86	2.19	3.051(11)	174
O2*W*—H2*WA*··· O5 ^{iii}	0.87	1.91	2.767(13)	172
O2*W*—H2*WB*··· O5 ^{iv}	0.87	2.37	3.106(11)	143
O3*W*—H3*WA*··· O3 ^{ii}	0.83	1.90	2.724(11)	170
O3*W*—H3*WB*··· O2 ^{v}	0.81	1.93	2.735(12)	170

Symmetry codes: (i) x+1/2, y+1/2, z; (ii) x, -y+1, z-1/2; (iii) x+1/2, -y+1/2, z+1/2; (iv) x+1/2, y-1/2, z; (v) x, y, z-1.