Electronic Supplementary Information

R-substituents Induced Structural diversity, Synergistic Effect and Highly selective Luminescence Sensing for Fe^{3+} Detection By Postsynthetically modified Cd-MOF

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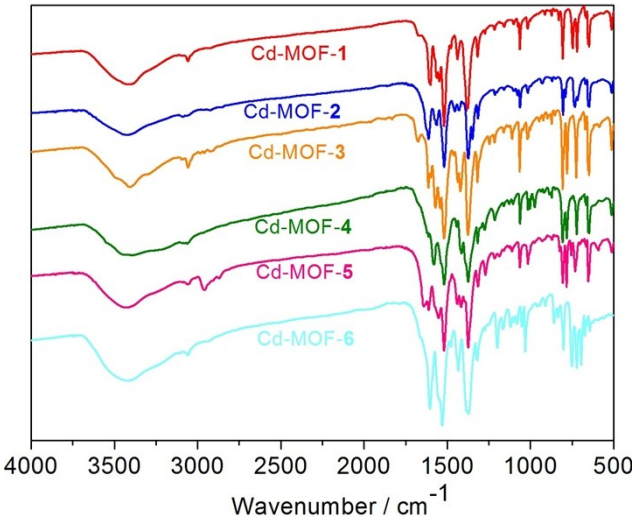

Fig.S1. The FT-IR spectra of the reported six Cd-MOFs in the present paper.

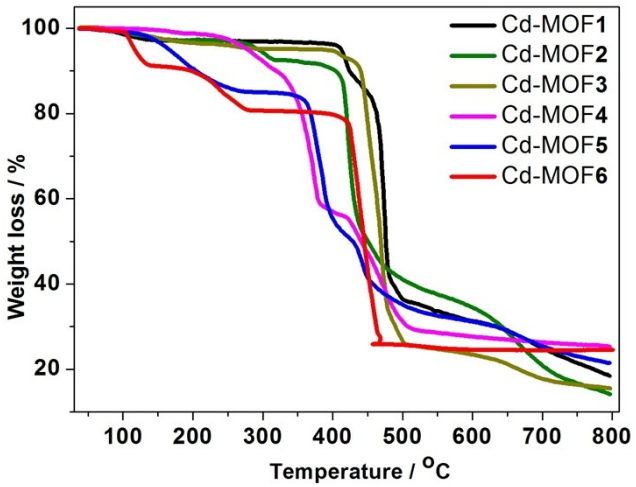

Fig. S2. The TGA curves for the reported six Cd-MOFs in the present paper. Upon heating, the samples started to lose the weight loss from room temperature. The first weitht loss (~3.6% for Cd-MOF-**1** and ~3.2% for Cd-MOF-**2**, ~4.9% for Cd-MOF-**3**, 14.9% for Cd-MOF-**5** and 8.9% for Cd-MOF-**6**) occured from room temperature, corresponding to the release of the guest water/DMF molecules (calculated loss 4.3% for Cd-MOF-**1** and ~5.4% for Cd-MOF-**2**, ~5.6% for Cd-MOF-**3**, 11.6% for Cd-MOF-**5** and 10.2% for Cd-MOF-**6**) in the structure. The further significant weight losses above about 380°C for Cd-MOF-**1**, **3** and **6**, 240°C for Cd-MOF-**2** and 330°C for Cd-MOF-**5** were due to the loss/decomposition of the ligands, showing the good thermal stabilities. For Cd-MOF-**4**, no evident platform on the TG curve was observed, even when the TGA experiment was done at slower heating rate (5 °C min^{-1}). In addition, the larger errors between the observed data and calculated data may arise from the moisture during the TGA experiments.

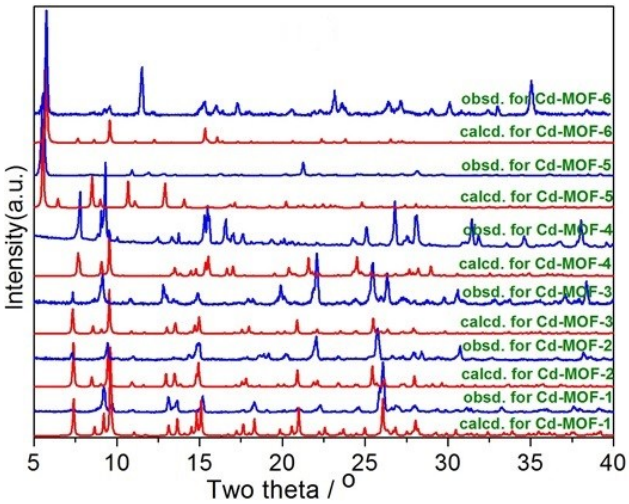

Fig.S3. The comparison of the observed and calculated PXRD patterns from the six Cd-MOFs.

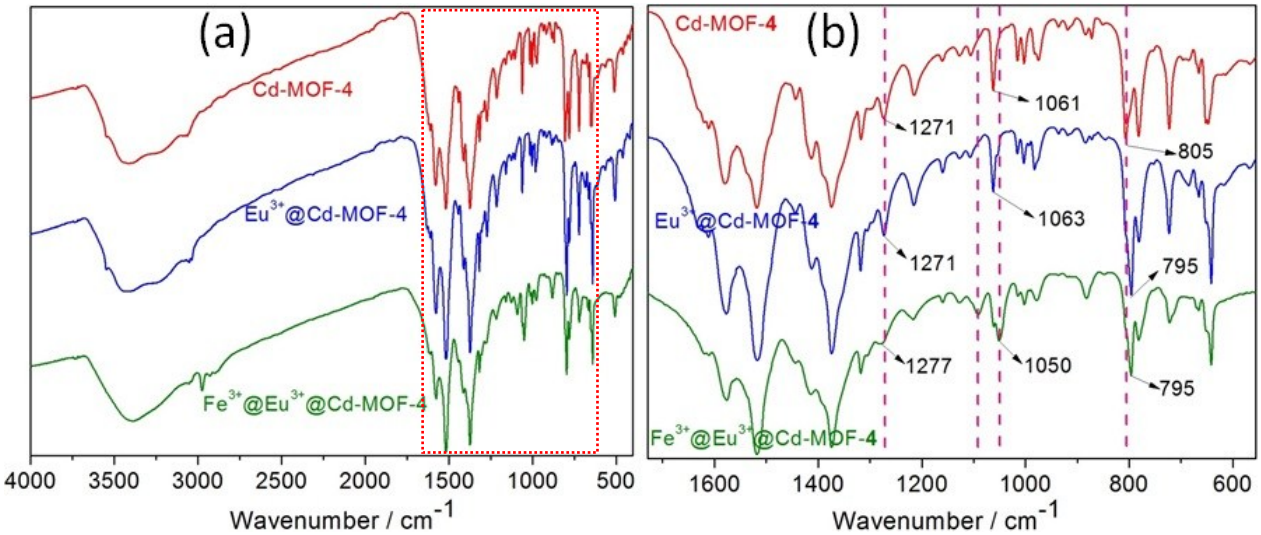

Fig. S4. (a) The FT-IR spectra of the as-synthesized Cd-MOF-**4**, Eu^{3+}@Cd-MOF-**4** and Fe^{3+}@Eu^{3+}@Cd-MOF-**4** samples; (b) the enlarged image highlighting the changes before and after the PSMs.

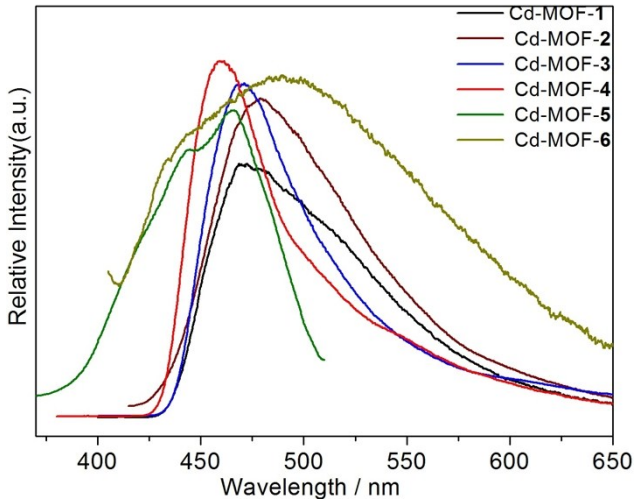

Fig.S5. The luminescence spectra of the reported six Cd-MOFs in the present paper.

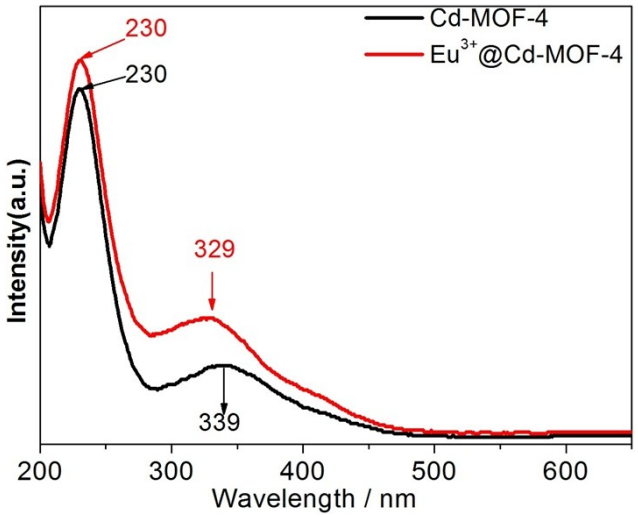

Fig. S6. The UV spectra of the Cd-MOF-4 and Eu^{3+}@Cd-MOF-**4**.

Table S1. Selected bond [Å] and angles [º] for compound **1-6**.

Cd1-O1	2.424(2)	Cd1-O2	2.324(2)
Cd1-O3A	2.234(2)	Cd1-O4B	2.302(2)
Cd1-N1	2.312(3)	Cd1-N2C	2.340(3)
O3A-Cd1-O4B	130.29(8)	O3A-Cd1-N1	91.27(9)
O4B-Cd1-N1	85.07(9)	O3A-Cd1-O2	143.95(9)
O4B-Cd1-O2	85.67(8)	N1-Cd1-O2	89.31(11)
O3A-Cd1-N2C	86.82(9)	O4B-Cd1-N2C	89.92(9)
N1-Cd1-N2C	171.59(9)	O2-Cd1-N2C	97.06(11)
O3A-Cd1-O1	90.23(8)	O4B-Cd1-O1	138.99(8)
N1-Cd1-O1	102.32(9)	O2-Cd1-O1	54.59(8)
N2C-Cd1-O1	85.89(9)		
Symmetry code for compound **1**: A x-1/2, y-1/2, z; B -x+1, -y+3, -z+1; C x+1/2, -y+5/2, z+1/2.			
Cd1-O1	2.338(3)	Cd1-O2	2.463(4)
Cd1-O3B	2.293(3)	Cd1-O4A	2.261(3)

Cd1-N1	2.301(3)	Cd1-N2C	2.321(3)
O1-Cd1-O2	54.39(11)	O4A-Cd1-N1	89.59(11)
O3B-Cd1-N1	88.53(12)	O4A-Cd1-N2C	85.15(12)
O3B-Cd1-N2C	88.21(12)	N1-Cd1-N2C	170.34(12)
O4A-Cd1-O1	98.38(11)	O3B-Cd1-O1	133.67(12)
N1-Cd1-O1	101.13(12)	N2C-Cd1-O1	87.67(12)
O4A-Cd1-O2	151.09(11)	O3B-Cd1-O2	81.47(11)
N1-Cd1-O2	87.03(13)	O4A-Cd1-O3B	127.16(12)
N2C-Cd1-O2	101.47(14)		
Symmetry codes for compound **2**: A x-1/2, y+1/2, z; B -x+1, -y, -z+1; C x+1/2, -y+1/2, z+1/2.			
Cd1-O1	2.236(3)	Cd1-O2A	2.291(3)
Cd1-N1	2.326(3)	Cd1-N3B	2.352(3)
Cd1-O3C	2.367(3)	Cd1-O4C	2.399(3)
O1-Cd1-O2A	126.96(12)	O1-Cd1-N1	90.77(12)
O2A-Cd1-N1	87.00(12)	O1-Cd1-N3B	85.84(12)
O2A-Cd1-N3B	88.16(12)	N1-Cd1-N3B	170.74(11)
O1-Cd1-O3C	148.87(12)	O2A-Cd1-O3C	84.11(11)
N1-Cd1-O3C	88.77(13)	N3B-Cd1-O3C	98.58(13)
O1-Cd1-O4C	95.54(11)	O2A-Cd1-O4C	136.74(11)
N1-Cd1-O4C	101.73(12)	N3B-Cd1-O4C	87.19(12)
O3C-Cd1-O4C	54.26(11)		
Symmetry code for compound **3**: A -x+1/2, -y+1/2, -z; B x-1/2, -y+1/2, z-1/2; C x-1/2, y+1/2, z.			
Cd1-O3A	2.211(3)	Cd1-O4B	2.228(3)
Cd1-N2C	2.327(3)	Cd1-O2	2.326(3)
Cd1-N1	2.352(3)	Cd1-O1	2.459(3)
O3A-Cd1-O4B	127.94(10)	O3A-Cd1-N2C	92.62(11)
O4B-Cd1-N2C	87.55(11)	O3A-Cd1-O2	85.33(10)
O4B-Cd1-O2	143.33(10)	N2C-Cd1-O2	108.14(10)
O3A-Cd1-N1	88.33(11)	O4B-Cd1-N1	85.56(11)
N2C-Cd1-N1	171.94(11)	O2-Cd1-N1	79.91(10)
O3A-Cd1-O1	139.75(10)	O4B-Cd1-O1	91.52(10)
N2C-Cd1-O1	97.24(10)	O2-Cd1-O1	54.51(10)
N1-Cd1-O1	87.13(10)		
Symmetry codes for compound **4**: A x-1/2, -y+1/2, z-1/2; B -x+1/2, y-1/2, -z+1/2; C x, -y, z-1/2.			
Cd1-N1	2.309(3)	Cd1-N2	2.400(3)
Cd1-O1A	2.263(3)	Cd1-O3B	2.485(3)
Cd1-O4B	2.252(3)	Cd1-O2	2.229(3)
O2-Cd1-O4B	144.52(10)	O2-Cd1-O1A	126.36(11)
O4B-Cd1-O1A	87.53(11)	O2-Cd1-N1	91.23(10)
O4B-Cd1-N1	97.15(11)	O1A-Cd1-N1	93.85(12)

O2-Cd1-N2	84.52(10)	O4B-Cd1-N2	88.52(11)
O1A-Cd1-N2	85.64(11)	N1-Cd1-N2	174.29(11)
O2-Cd1-O3B	91.98(10)	O4B-Cd1-O3B	54.89(10)
O1A-Cd1-O3B	141.66(10)	N1-Cd1-O3B	84.69(13)
N2-Cd1-O3B	99.23(13)		
Symmetry code for compound **5**: A -x+5/3,-y-2/3,-z+4/3; B y+4/3,-x+y+2/3,-z+5/3.			
Cd1-O1	2.402(4)	Cd1-O2	2.356(4)
Cd1-O3A	2.267(4)	Cd1-O4B	2.296(4)
Cd1-N1	2.325(5)	Cd1-N2	2.302(5)
O3A-Cd1-O4B	123.09(13)	O3A-Cd1-N2	89.19(17)
O4B-Cd1-N2	94.91(16)	O3A-Cd1-N1	81.91(17)
O4B-Cd1-N1	86.50(17)	N2-Cd1-N1	170.16(16)
O3A-Cd1-O2	144.53(15)	O4B-Cd1-O2	92.37(14)
N2-Cd1-O2	88.32(16)	N1-Cd1-O2	101.37(16)
O3A-Cd1-O1	90.81(14)	O4B-Cd1-O1	144.67(14)
N2-Cd1-O1	95.22(17)	N1-Cd1-O1	89.14(17)
O2-Cd1-O1	54.25(14)		
Symmetry code for compound **6**: A y+1/3, x-1/3, -z+1/6; B -y+1/3, -x+2/3, z+1/6.			