Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information for the Manuscript:

Anionic Porous Metal–Organic Framework with Novel 5-Connected vbk Topology for Rapid Adsorption of Dyes and Tunable White Light Emission

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Table S1 Crystal data and structure refinement for Zn(II)-MOF.

Identification code	Zn(II)-MOF
formula	$C_{50}H_{32}O_{27}Zn_4$
fw	1326.24
Crystal system	$P2_1/c$
Space group	Monoclinic
a (Å)	17.493(4)
b (Å)	15.092(3)
c (Å)	23.745(5)
α (°)	90
β (°)	97.06(3)
γ (°)	90
V (Å^3)	6221(2)
Z	2
Dc (Mg·m^3)	0.708
F(000)	1336
Reflns collected	41060
Independent reflns	10884
R(int)	0.0315
GOF on F^2	1.449
$R_1{}^a$ ($I>2\sigma$ (I))	0.0962
$wR_2{}^b$ ($I>2\sigma(I)$)	0.3157

$^aR_1 = \sum||F_o|-|F_c||/\sum|F_o|$. $^bwR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

Table S2. Selected bond distances and angles for Zn(II)-MOF[a].

Zn(1)-O(1)	1.901(3)	Zn(1)-O(3)#1	1.911(5)
Zn(1)-O(8)#2	1.917(3)	Zn(1)-O(10)#3	1.948(5)
Zn(2)-O(2)	1.949(3)	Zn(2)-O(6)#4	1.963(3)
Zn(2)-O(9)#3	1.972(4)	Zn(2)-O(4)#1	2.079(5)
Zn(2)-O(1W)	2.172(6)	O(1)-Zn(1)-O(3)#1	116.0(2)
O(1)-Zn(1)-O(8)#2	115.16(15)	O(3)#1-Zn(1)-O(8)#2	107.97(19)
O(1)-Zn(1)-O(10)#3	111.7(2)	O(3)#1-Zn(1)-O(10)#3	105.1(2)
O(8)#2-Zn(1)-O(10)#3	99.19(17)	O(2)-Zn(2)-O(6)#4	109.53(14)
O(2)-Zn(2)-O(9)#3	142.23(14)	O(6)#4-Zn(2)-O(9)#3	107.79(15)
O(2)-Zn(2)-O(4)#1	93.58(18)	O(6)#4-Zn(2)-O(4)#1	91.14(17)
O(9)#3-Zn(2)-O(4)#1	91.3(2)	O(2)-Zn(2)-O(1W)	84.0(2)
O(6)#4-Zn(2)-O(1W)	96.8(2)	O(9)#3-Zn(2)-O(1W)	86.1(2)
O(4)#1-Zn(2)-O(1W)	172.09(19)		

[a]Symmetry transformations used to generate equivalent atoms: #1 *X*, -*Y*+3/2, *Z*+1/2; #2 -*X*, -*Y*+1, -*Z*+1; #3 *X*, *Y*+1, *Z*; #4 –*X*+1, *Y*+1/2, -*Z*+1/2; #5 *X*, -*Y*+3/2, *Z*-1/2; #6 –*X*+1, *Y*-1/2, -*Z*+1/2; #7 *X*, *Y*-1, *Z*.

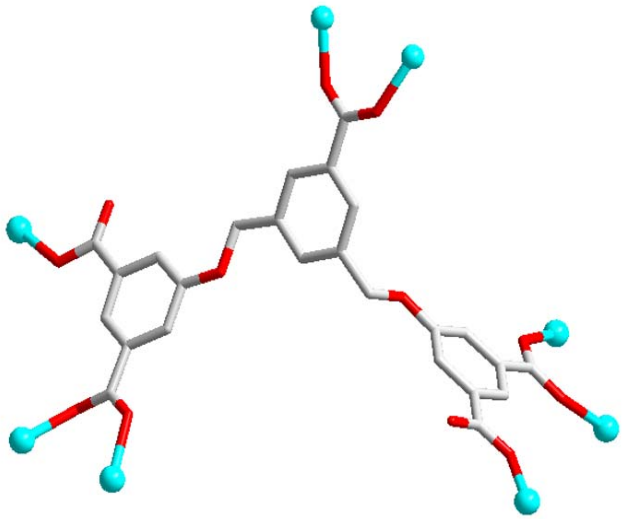

Fig. S1 Coordination Mode of the L^{5-} Anion.

Fig. S2 The "paddle-wheel" secondary building unit (SBU).

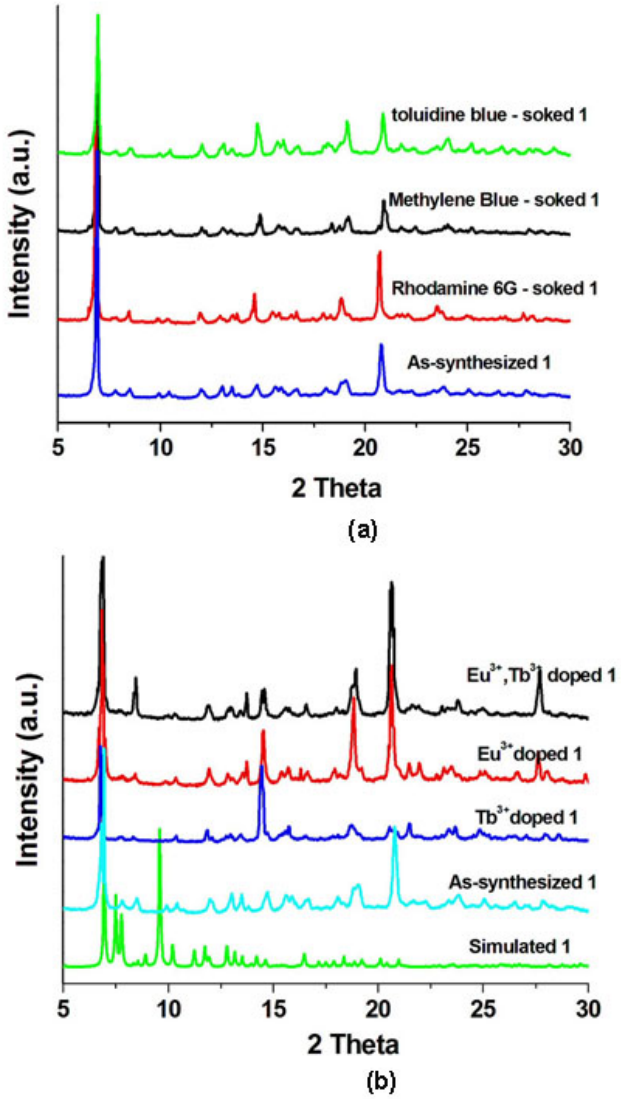

Fig. S3 Powder XRD patterns for simulated, as-synthesized, lanthanide cations-doped Zn(II)-MOF and dye-soaked Zn(II)-MOF.

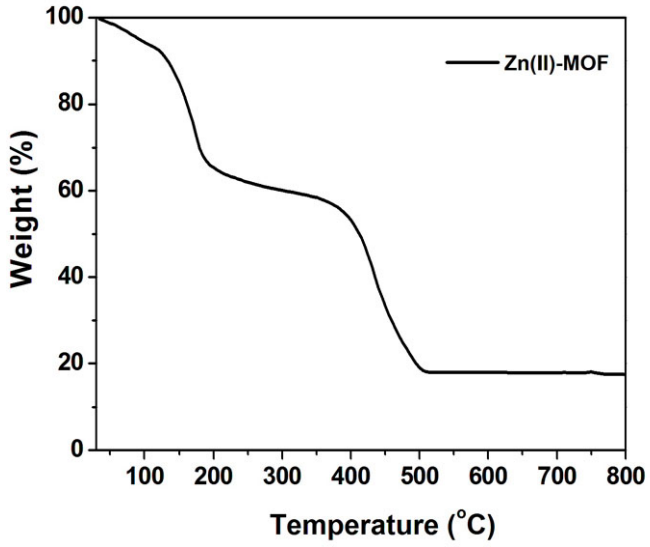

Fig. S4 The thermogravimetric (TG) analysis curve of Zn(II)-MOF.

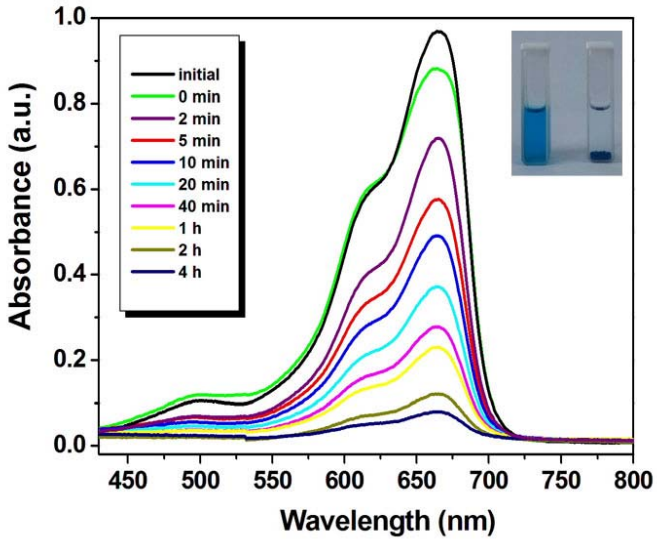

Fig. S5 UV–vis spectra of the original and Zn(II)-MOF treated (30 mg) organic dye MB (5.0×10^{-5} M) solution for various times. The insets are photos before and after the adsorption experiments under sunlight.

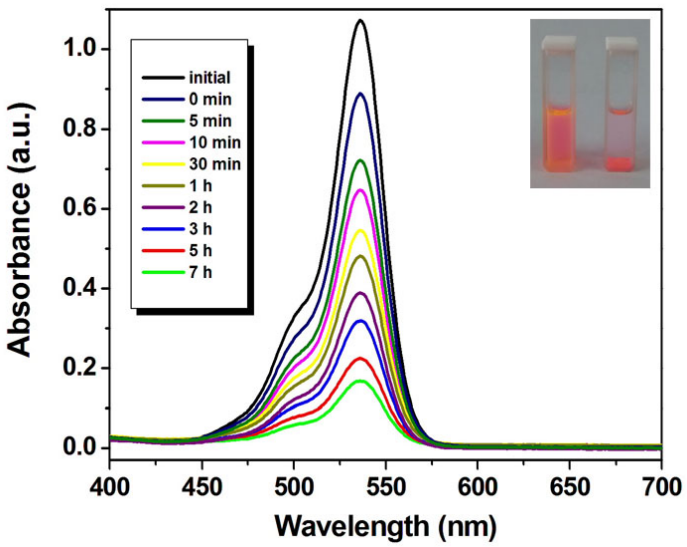

Fig. S6 UV–vis spectra of the original and Zn(II)-MOF treated (30 mg) organic dye R6G (5.0×10^{-5} M) solution for various times. The insets are photos before and after the adsorption experiments under sunlight.

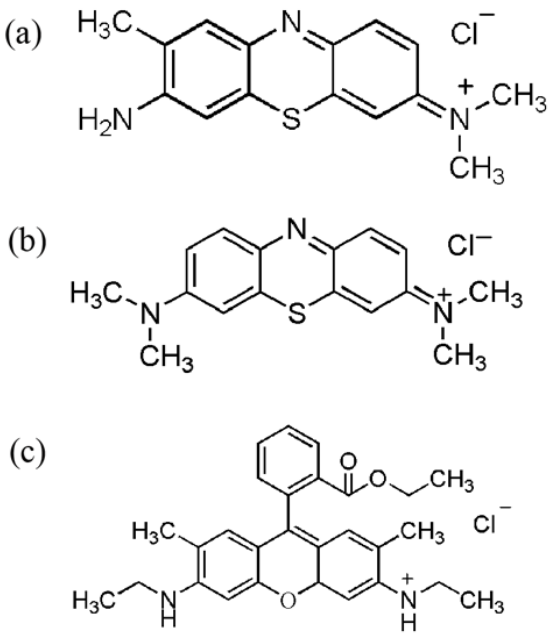

Fig. S7 Molecular structures of (a) TB, (b) MB, (c) R6G.

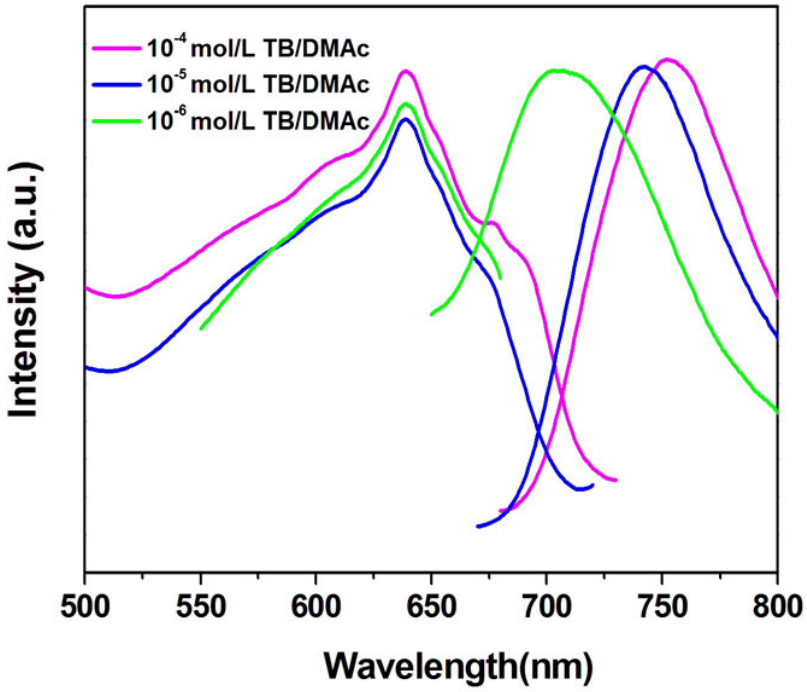

Fig. S8 Fluorescence spectra of Zn(II)-MOF dipped in different amounts of Toluidine Blue (TB) dye molecules.

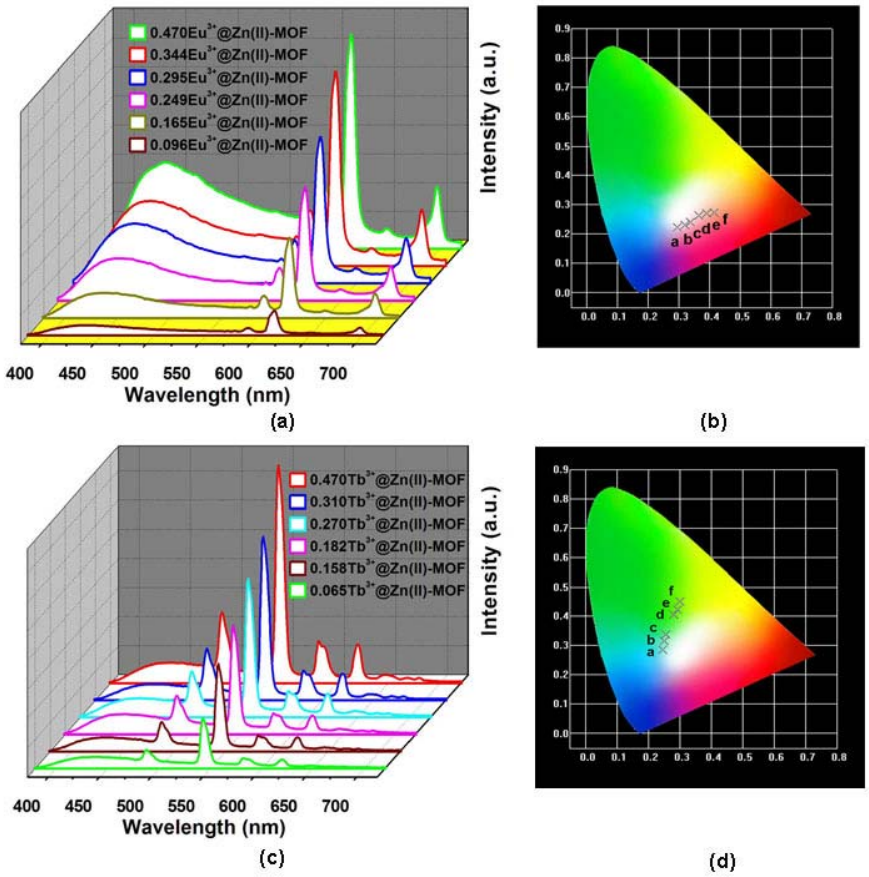

Fig. S9 (a) Emission spectra of xEu^{3+}@Zn(II)-MOF excitation at 359 nm. (b) CIE chromaticity coordinates and optical photographs of xEu^{3+}@Zn(II)-MOF. (c) Emission spectra of xTb^{3+}@Zn(II)-MOF excitation at 359 nm. (d) CIE chromaticity coordinates and optical photographs of xTb^{3+}@Zn(II)-MOF.

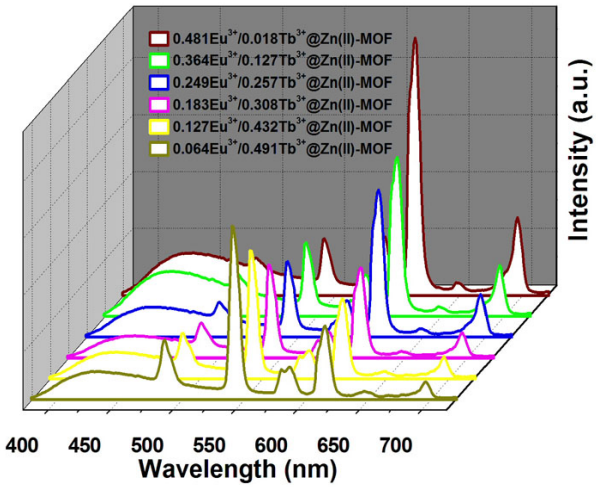

Fig. S10 The emission spectra of xEu^{3+}, yTb^{3+}@Zn(II)-MOF excitation at 359 nm.