Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Dimensional expansion of 1D zigzag chains to a 2D two-fold interpenetrated Metal-Organic Framework for adsorption of lanthanide cations and white light emission

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Table S1. Crystallographic data and refinement details for HSB-W10.

Name	HSB-W10
Empirical formula	$C_{22}H_{31}N_4O_8Cd$
M	591.91
Crystal system	triclinic
Space group	*P-1*
a (Å)	9.7448(3)
b (Å)	11.2596(3)
c (Å)	14.0846(4)
α (°)	68.021(3)
β (°)	84.398(2)
γ (°)	66.219(3)
V/Å^3	1308.81(8)
Z	2
ρ_{calc} (g/cm^{-3})	1.502
μ/mm^{-1}	4.832
2θ $_{range}$(°)	5.894 to 105.862
h, k, l, ranges	-11 to 10, -13 to 11, -16 to 16
F(000)	606.0
R1,[a]wR_2[b][I > 2σ(I)]	0.0432, 0.1149
GOF on F^2	1.053

[a] $R = \Sigma(||Fo| - |Fc||)/\Sigma|Fo|$. [b]$Rw = \{\Sigma w[(Fo^2 - Fc^2)^2]/\Sigma w[(Fo^2)^2]\}^{1/2}$.

Table S2. Selected bond lengths (Å) and angles(°) of HSB-W10.

Cd1[a]-O1[a]	2.198(3)
Cd1[a]-O4[a]	2.435(3)
Cd1[a]-N1[a]	2.358(3)
Cd1[a]-N2[a]	2.338(4)
Cd1[a]-N4[b]	2.377(3)
Cd1[a]-C19[a]	2.734(4)
O3[a]-Cd1[a]- O4[a]	54.72(9)
O4[a]-Cd1[a]-C19[a]	27.71(11)
O1[a]-Cd1[a]-O3[a]	97.13(12)
O1[a]-Cd1[a]-O4[a]	150.51(12)

$O1^{a}$-$Cd1^{a}$-$N4^{c}$	87.10(12)
$O1^{a}$-$Cd1^{a}$-$N1^{a}$	98.97(13)
$O1^{a}$-$Cd1^{a}$-$C19^{a}$	123.20(13)
$O1^{a}$-$Cd1^{a}$-$N2^{a}$	114.69(15)
$N4^{c}$-$Cd1^{a}$-$O3^{a}$	86.93(11)
$N4^{c}$-$Cd1^{a}$-$O4^{a}$	83.10(10)
$N4^{c}$-$Cd1^{a}$-$C19^{a}$	81.35(11)
$N1^{a}$-$Cd1^{a}$-$O3^{a}$	94.49(11)
$N1^{a}$-$Cd1^{a}$-$O4^{a}$	92.55(11)
$N1^{a}$-$Cd1^{a}$-$N4^{c}$	173.52(12)
$N1^{a}$-$Cd1^{a}$-$C19^{a}$	97.03(12)
$N2^{a}$-$Cd1^{a}$-$O3^{a}$	148.09(13)
$N2^{a}$-$Cd1^{a}$-$O4^{a}$	94.08(12)
$N2^{a}$-$Cd1^{a}$-$N4^{c}$	96.55(13)
$N2^{a}$-$Cd1^{a}$-$N1^{a}$	78.93(14)
$N2^{a}$-$Cd1^{a}$-$C19^{a}$	121.79(14)

Symmetry codes: (a) x, y, z; (b) 1+x, +y, +z; (c) 1+x, +y, +z.

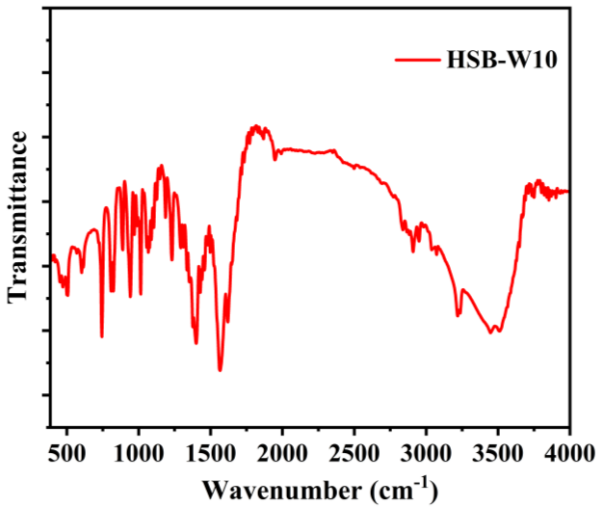

Figure S1. FT-IR spectra of HSB-W10.

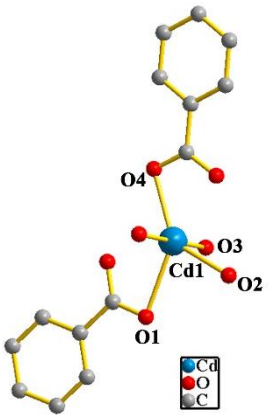

Figure S2. View of the coordination environment of Cd(II) ion in Cd-bdc (hydrogen atoms and free water molecules have been omitted for clarity).

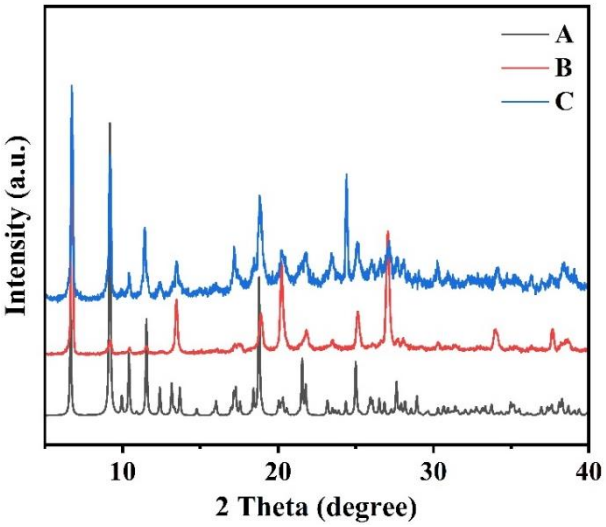

Figure S3. PXRD patterns of simulated HSB-W10 (A), dispersed bulk HSB-W10 (B) and clustered HSB-W10 (C).

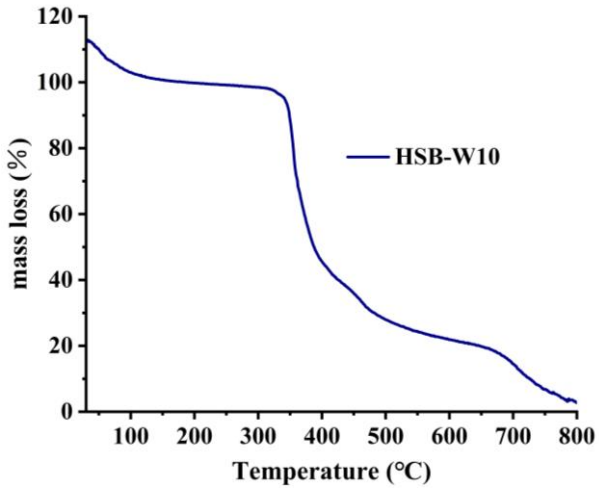

Figure S4. TGA plots for HSB-W10.

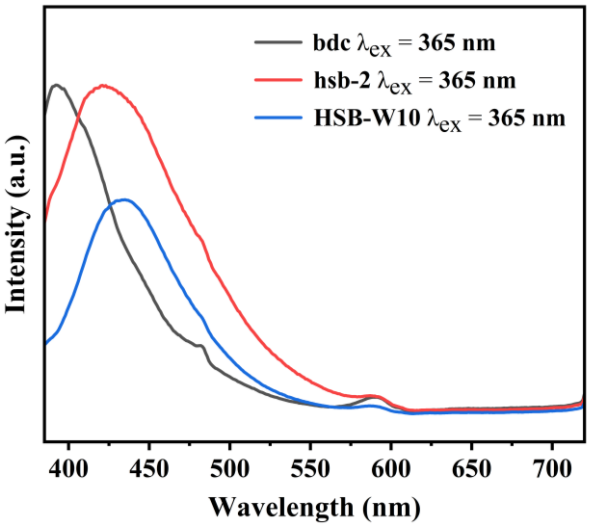

Figure S5. Emission spectra of bdc, hsb-2 and HSB-W10 with excitation wavelength (λ_{ex}) of 365 nm

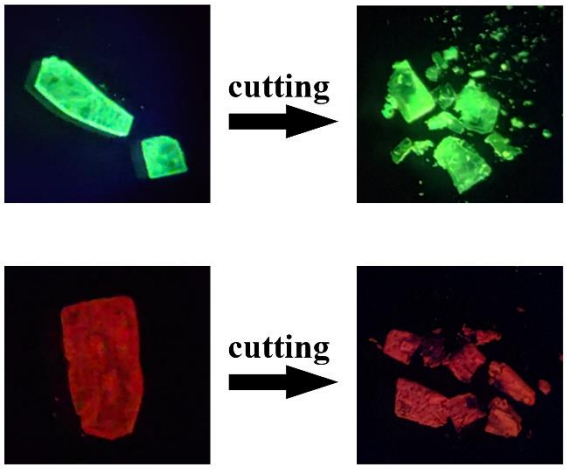

Figure S6. The photographs of crystals $Tb(H_2O)_x^{3+}$@HSB-W10 and $Eu(H_2O)_x^{3+}$@HSB-W10, and their pieces irradiated by a standard 254 nm laboratory UV lamp.

Table S3. The amounts of Eu^{3+} in $Eu(H_2O)_x^{3+}$@HSB-W10 composites based on ICP measurement.

Composite name $xEu(H_2O)_x^{3+}$@HSB-W10	Initial concentration of Eu^{3+} (mol L^{-1})	Amount of Cd^{2+} (%)	Amount of Eu^{3+} (%)
$0.024Eu(H_2O)_x^{3+}$@HSB-W10	0.009	15.94	0.52
$0.042Eu(H_2O)_x^{3+}$@HSB-W10	0.018	17.97	1.02
$0.04Eu(H_2O)_x^{3+}$@HSB-W10	0.027	17.48	0.96

Table S4. The amounts of Tb^{3+} in $Tb(H_2O)_8^{3+}$@HSB-W10 composites based on ICP measurement.

Composite name $xTb(H_2O)_x^{3+}$@HSB-W10	Initial concentration of Tb^{3+} (mol L^{-1})	Amount of Cd^{2+} (%)	Amount of Tb^{3+} (%)
$0.021Tb(H_2O)_x^{3+}$@HSB-W10	0.006	16.44	0.49
$0.024Tb(H_2O)_x^{3+}$@HSB-W10	0.012	16.16	0.55
$0.03Tb(H_2O)_x^{3+}$@HSB-W10	0.018	15.50	0.64

Table S5. The amounts of Eu^{3+} and Tb^{3+} in WLE $Eu(H_2O)_x^{3+}/Tb(H_2O)_x^{3+}$@HSB-W10 composites based on ICP measurement.

Composite name $xTb(H_2O)_x^{3+}/yEu(H_2O)_x^{3+}$@HSB-W10	Amount of Cd^{2+} (%)	Amount of Eu^{3+} (%)	Amount of Tb^{3+} (%)
$0.064Tb(H_2O)_x^{3+}/0.012Eu(H_2O)_x^{3+}$@HSB-W10	14.91	0.25	1.34

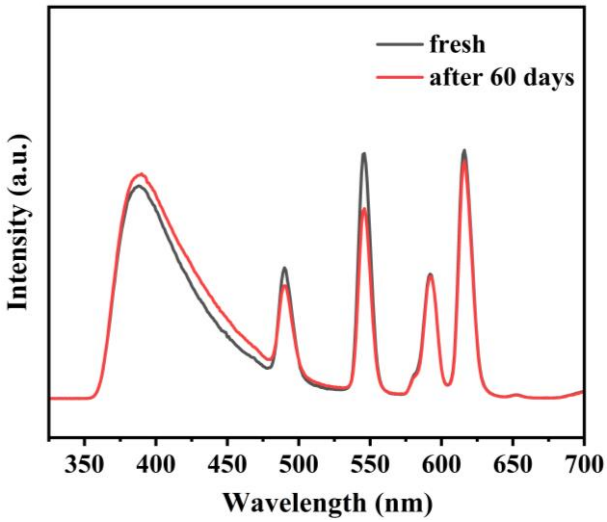

Figure S7. Comparation of the emission spectra of 0.064Tb$(H_2O)_x^{3+}$/0.012 Eu$(H_2O)_x^{3+}$@HSB-W10 (fresh vs. after 60 days).