Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

An ideal detector composed of a 3D Gd-based coordination ploymer for DNA and Hg^{2+} ion

Shu-Na Zhao,[a,b] Lan-Lan Wu, [a,b] Jing Feng, [a] Shu-Yan Song,*[a] and Hong-Jie Zhang*[a]

[a]State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, 5625 Renmin Street, Changchun, 130022 (P.R. China)

[b]University of Chinese Academy of Sciences, Beijing, 100049 (P.R. China)

*Corresponding author

Email: songsy@ciac.ac.cn (Shu-Yan Song); hongjie@ciac.ac.cn (Hong-Jie Zhang)

Tel: 86-431-85262127.

Fax: 86-431-85698041.

Table S1. Crystal data and structure refinements of compound GdL

Compound	GdL
formula	$GdC_{11}H_6N_3O_6$
fw	433.44
T/K	296(2)
λ (Mo Kα), Å	0.71073
cryst syst	monoclinic
space group	$P2_1/n$
a (Å)	7.7512(12)
b (Å)	8.0176(13)
c (Å)	18.399(3)
α (deg)	90
β (deg)	96.125(2)
γ (deg)	90
V/Å^3	1136.9(3)
Z	4
$D_{calcd.}$(g·cm^{-3})	2.532
F(000)	820
$2\theta_{max}$ (°)	50.18
GOF	1.035
R_1(I > 2σ(I))[a]	0.0258
wR_2[b](all data)	0.0526

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma(|F_o|^2 - |F_c|^2)/\Sigma|F_o|^2]^{1/2}$.

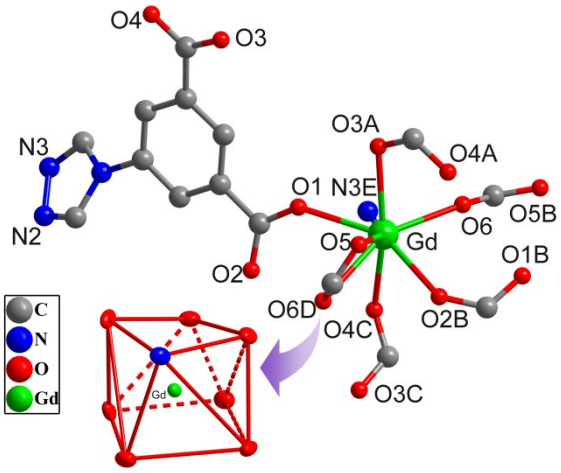

Fig. S1 Local coordination environment of the GdIII ions in GdL. Hydrogenatoms attached to carbon atoms are omitted for clarity. Symmetry codes: A:-x, -y, -z; B:0.5-x, 0.5+y, 0.5-z; C:0.5+x, -0.5-y, 0.5+z; D:0.5-x, -0.5+y, 0.5-z; E:1-x, -1-y, -z.

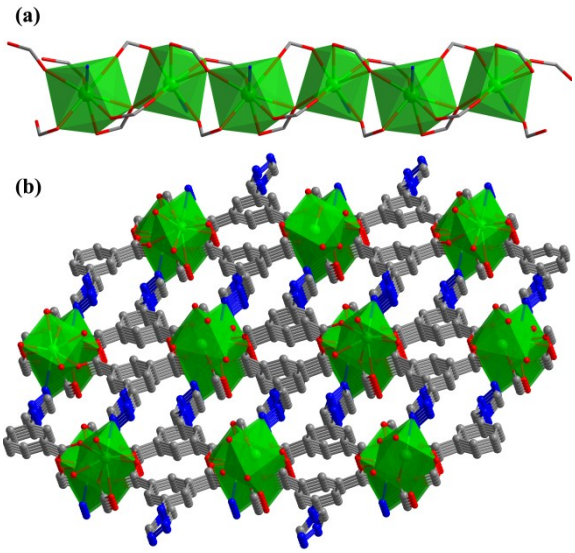

Fig. S2 (a) Infinite 1D chains; (b) The 3D framework of GdL.

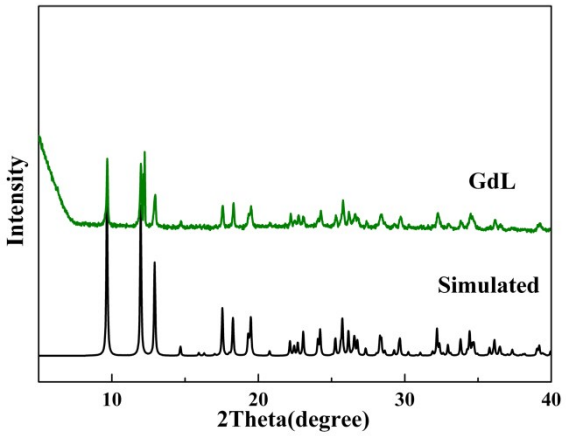

Fig. S3 Power X-ray diffraction pattern of simulated and experimental as-synthesized compound GdL.

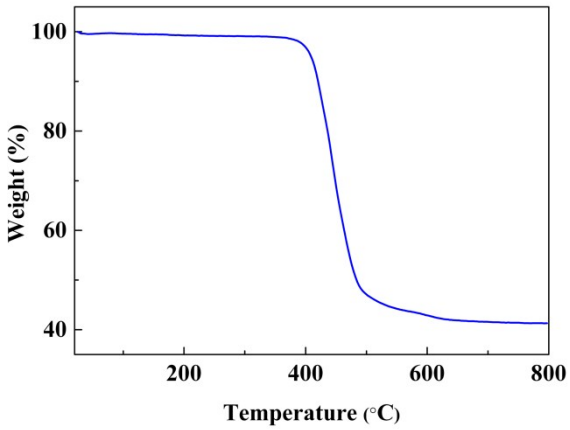

Fig. S4 TGA curve of compounds GdL.

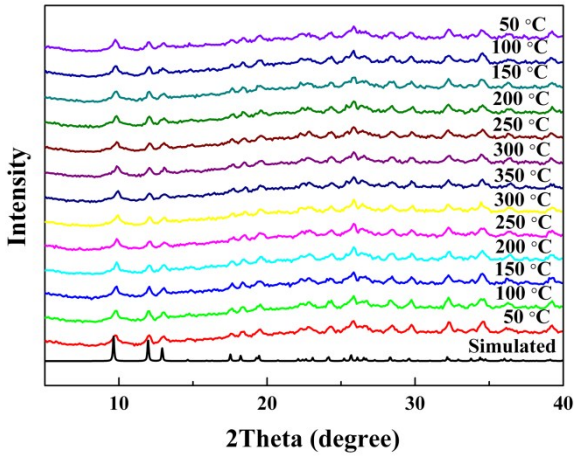

Fig. S5 Power X-ray diffraction pattern of simulated and experimental as-synthesized compound GdL from 50 °C to 350 °C, then from 350 °C to 50 °C.

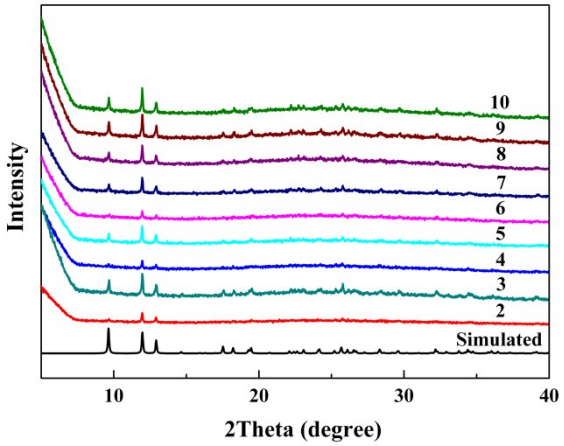

Fig. S6 Power X-ray diffraction pattern of compound GdL after being immersed in the solution of pH = 2-10 for two weeks.

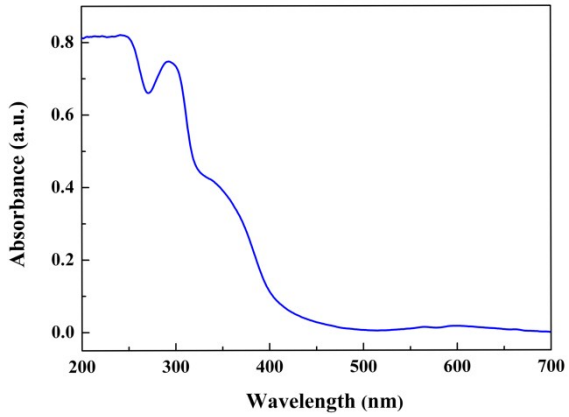

Fig. S7 The UV-Vis diffuse reflectance spectra (DRS) of GdL.

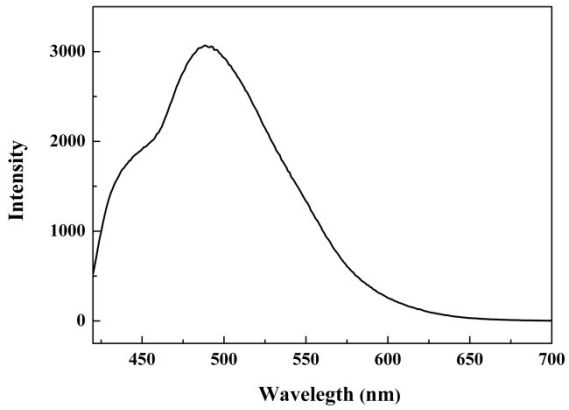

Fig. S8 Room-temperature emission spectra for GdL in the solid state excited at 405

nm.

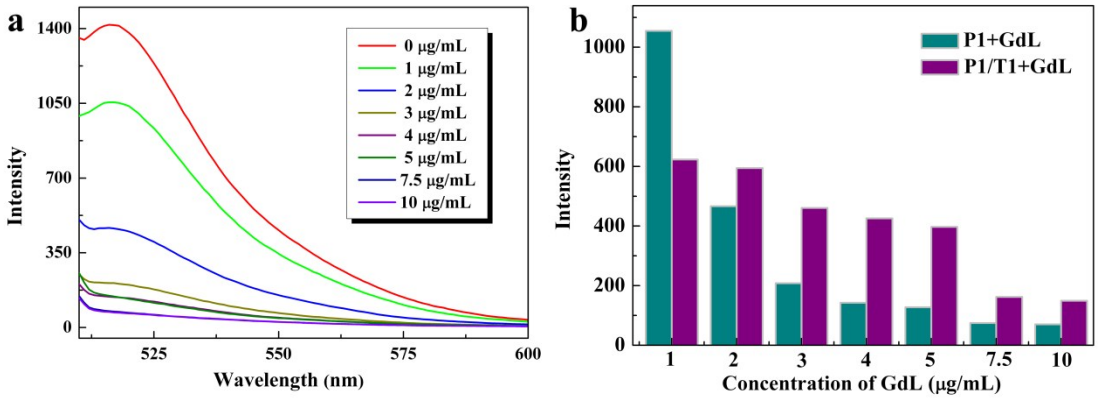

Fig. S9 (a) Fluorescence emission spectra of P1 in Tris-HCl buffer in the presence of different concentrations of GdL (from top to bottom: 0, 1, 2, 3, 4, 5, 7.5 and 10 μg/mL); (b) Influence of the amount of GdL (green column) or T1 (violet column) on the fluorescence quenching efficiency. (P1: 50 nM; T1: 50 nM; pH: 7.4 in the Tris-HCl buffer)

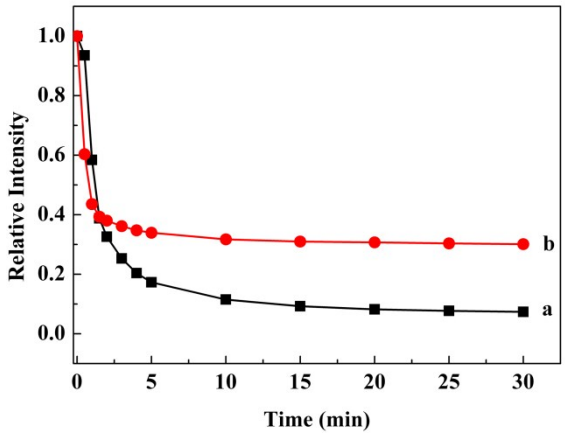

Fig. S10 The fluorescence quenching curves for P1 (50 nM)/MOF (5 μg/mL) composite as a function of time (a) in the absence of T1 and (b) in the presence of T1 of 50 nM. The excitation and emission wavelengths are 494 and 517 nm.

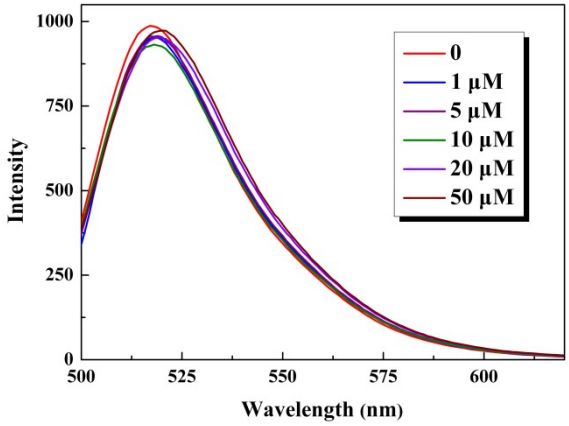

Fig. S11 The fluorescence emission spectrum of P2 in the presence of Hg^{2+} from 0 to 50.0 μM in Tris-HCl buffer. Excitation was at 480 nm.

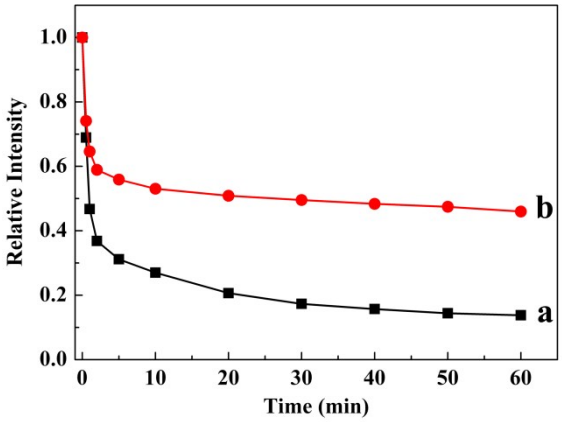

Fig. S12 The fluorescence quenching curves for P2 (100 nM)/MOF (20 μg/mL) composite as a function of time (a) in the absence of Hg^{2+} and (b) in the presence of Hg^{2+} of 10 μM. The excitation and emission wavelengths are 480 and 517 nm.

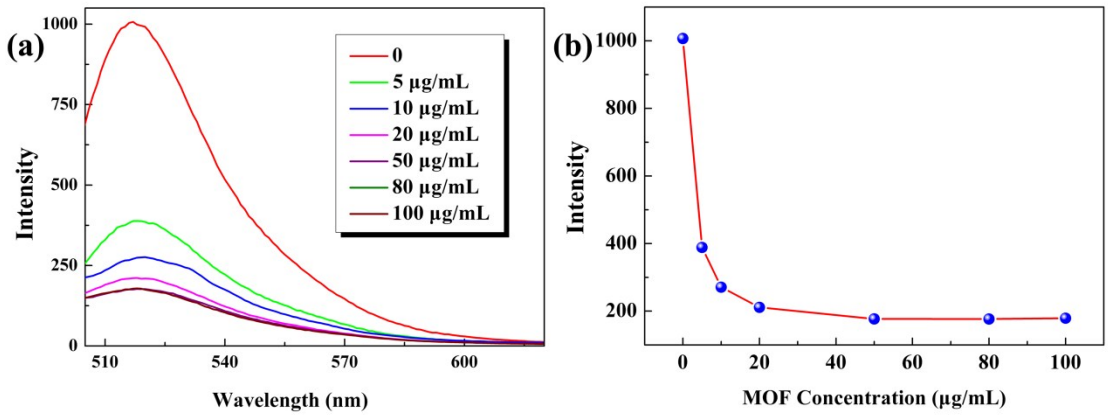

Fig. S13 (a) Fluorescence emission spectra of P2 in Tris-HCl buffer in the presence of

different concentration of GdL (from top to bottom: 0, 5, 10, 20, 50, 80 and 100 μg/mL); (b) the corresponding fluorescence intensity at 517 nm wavelength plotted against GdL concentration. Excitation was at 480 nm and fluorescence intensity was recorded at 517 nm.

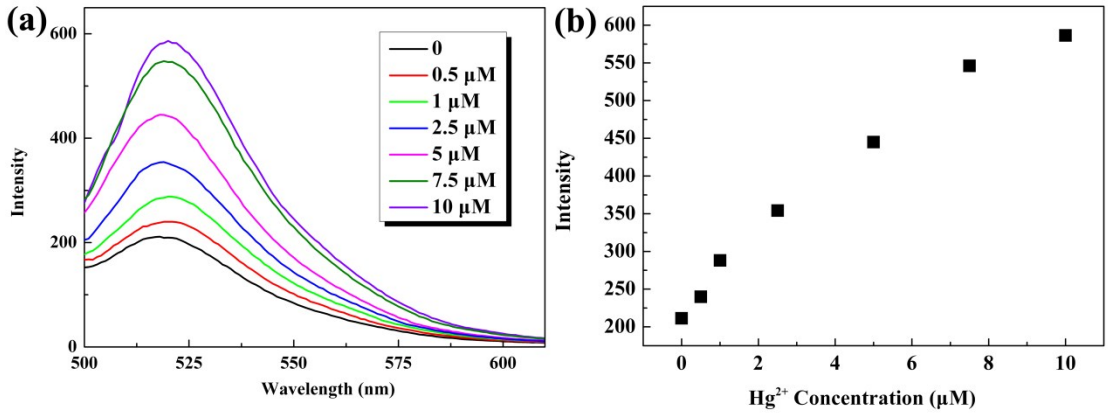

Fig. S14 (a) Fluorescence spectra of P2/GdL in the presence of different concentrations of Hg^{2+} in Tris-HCl buffer (pH = 7.4) (from bottom to top: 0, 0.5, 1, 2.5, 5, 7.5, and 10 μM). Excitation was at 480 nm and emission intensity was recorded at 517 nm; (b) the corresponding fluorescence intensity plotted against Hg^{2+} concentration.