Supplementary Information

A multifunctional colorimetric sensors originated from a cadmium naphthalene diimide-based metal-organic framework: photochromism, hydrochromism and vapochromism

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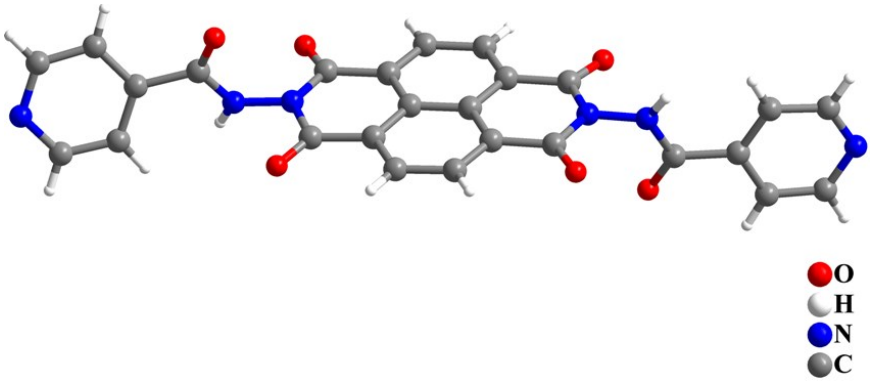


Fig. S1. The structure of N,N′-di(4-pyridylacylamino)-1,4,5,8-naphthalenediimide (IsoNDI)

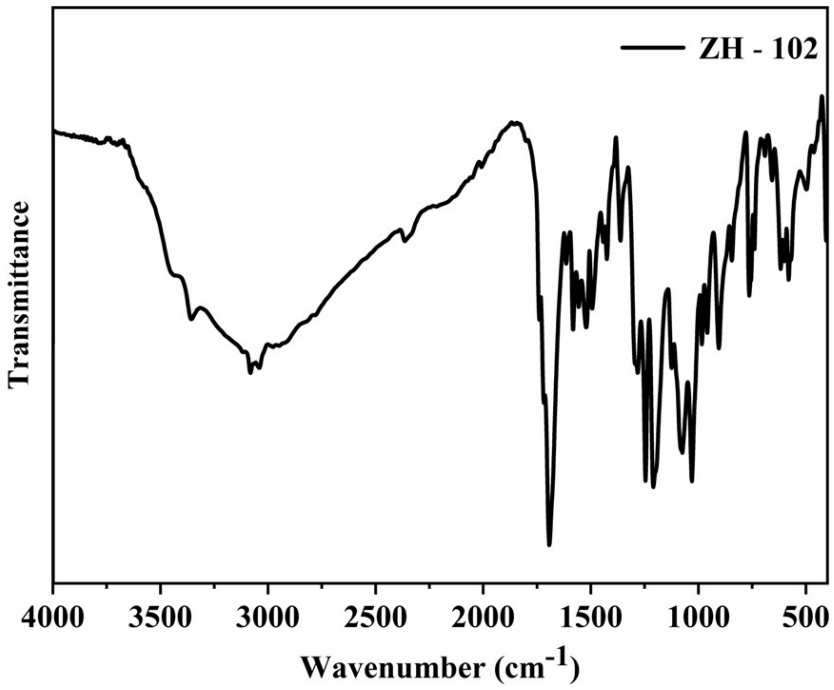
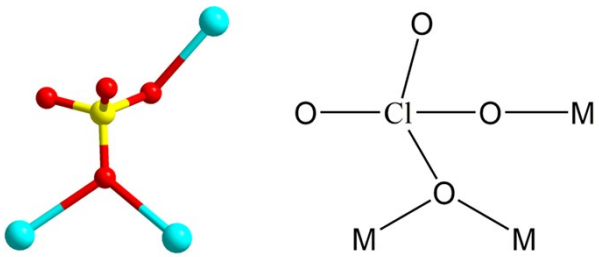


Fig. S2. FT-IR spectra of compound **ZH-102**.



[3.2100]

Fig. S3. The Harris notation of the **ZH-102**.

Table S1. The selected bond lengths [Å] and angles [º] of complex **ZH-102.**

Cd(1)-O(8)	2.258(2)	Cd(1)-N(4)#2	2.356(2)
Cd(1)-N(3)	2.304(2)	Cd(1)-O(7)	2.357(2)
Cd(1)-O(11)#1	2.3072(18)	Cd(1)-O(11)#3	2.3811(18)
O(8)-Cd(1)-N(3)	107.96(8)	N(3)-Cd(1)-O(7)	86.07(8)
O(8)-Cd(1)-O(11)#1	95.82(7)	O(11)#1-Cd(1)-O(7)	176.62(7)
N(3)-Cd(1)-O(11)#1	92.18(7)	N(4)#2-Cd(1)-O(7)	83.89(8)
O(8)-Cd(1)-N(4)#2	83.50(8)	O(8)-Cd(1)-O(11)#3	163.70(7)
N(3)-Cd(1)-N(4)#2	164.42(8)	N(3)-Cd(1)-O(11)#3	85.03(7)
O(11)#1-Cd(1)-N(4)#2	97.21(8)	O(11)#1-Cd(1)-O(11)#3	73.37(7)
O(8)-Cd(1)-O(7)	87.48(8)	N(4)#2-Cd(1)-O(11)#3	85.79(7)
O(7)-Cd(1)-O(11)#3	103.57(7)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+2, #2 x-1,y-1,z+1, #3 x+1,y,z, #4 x-1,y,z, #5 x+1,y+1,z-1.

Band	Distance	r_o	Value
CD1 – O7	2.360(3)	1.904	0.291
CD1 – O8	2.254(3)	1.904	0.388
CD1 – O11#1	2.306(2)	1.904	0.337
CD1 – O11#3	2.379(2)	1.904	0.277
CD1 – N3	2.301(3)	1.960	0.398
CD1 – N4#2	2.352(3)	1.960	0.347
Valence			2.038

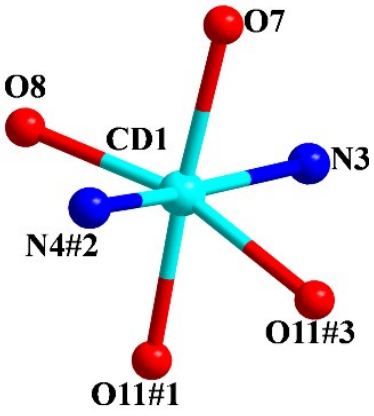


Fig. S4. BVS and coordination mode for the site Cd1 in the **ZH-102.**

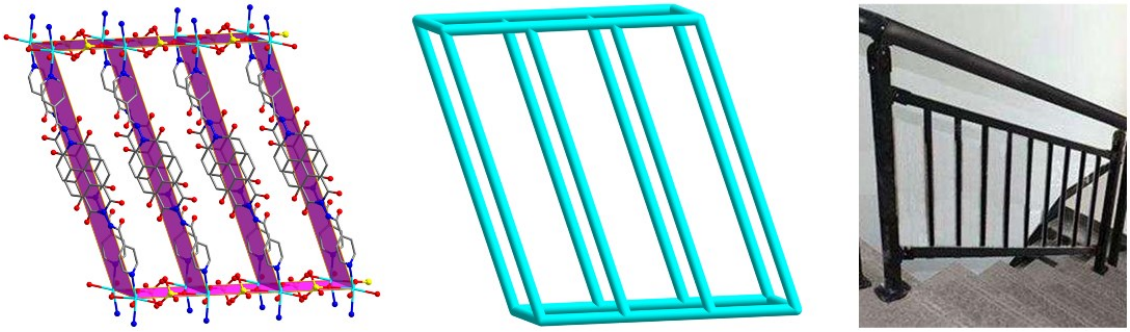


Fig. S5. A structure similar to a ‘safety fence’ of the **ZH-102**.

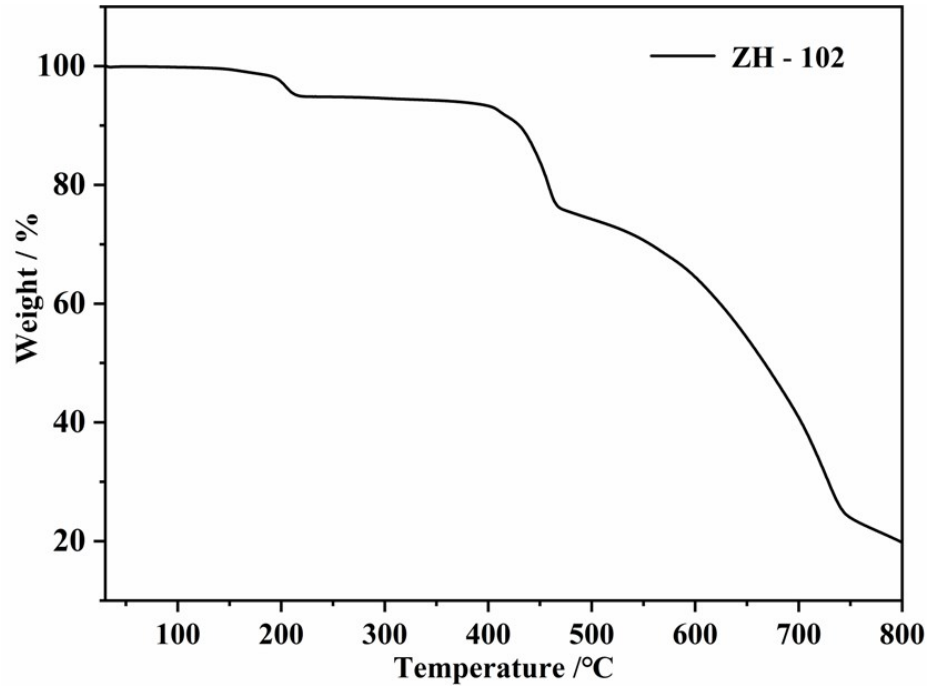


Fig. S6. TG curves for compound **ZH-102**.

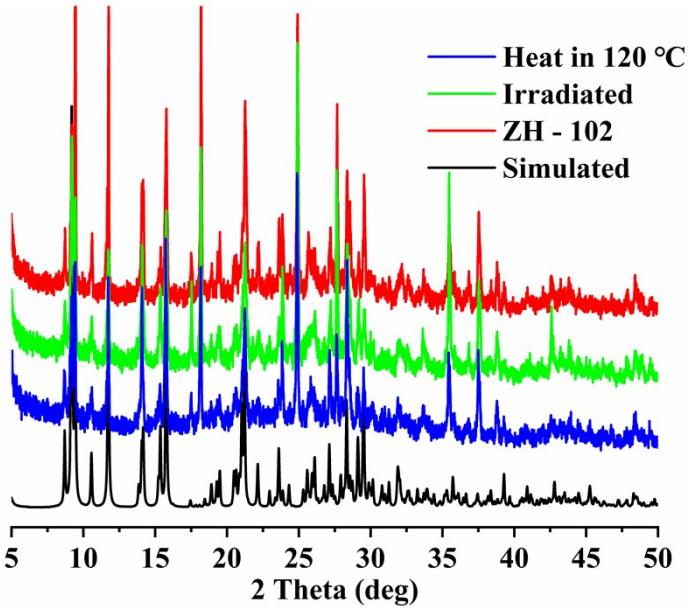


Fig. S7. PXRD patterns of the **ZH-102**; the simulated, as-synthesized (**ZH-102**), the irradiated crystals and the irradiated crystals after heated 120 ℃.

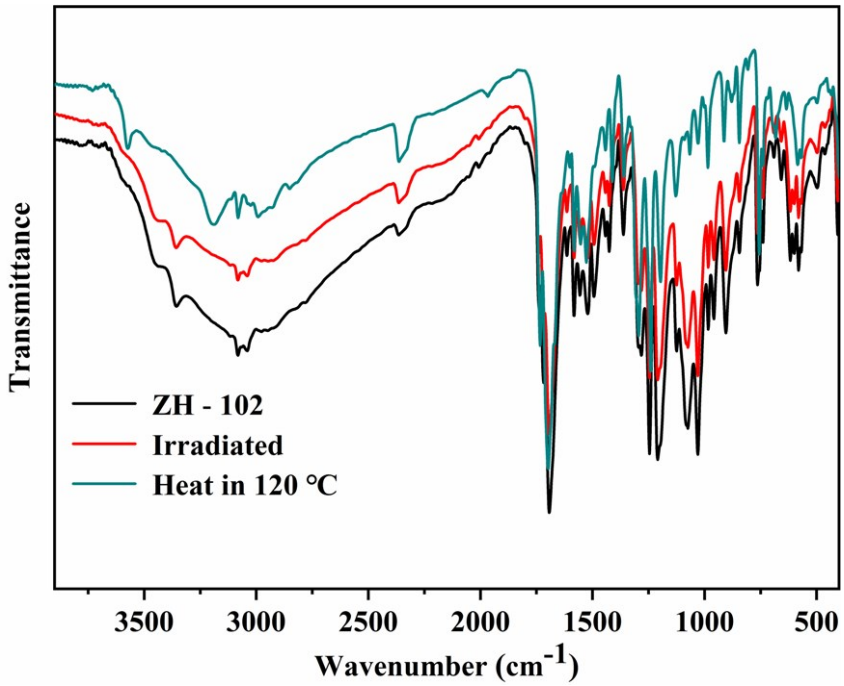


Fig. S8. IR spectra of the **ZH-102**; as-synthesized (**ZH-102**), the irradiated crystals and the irradiated crystals after heated 120 ℃.

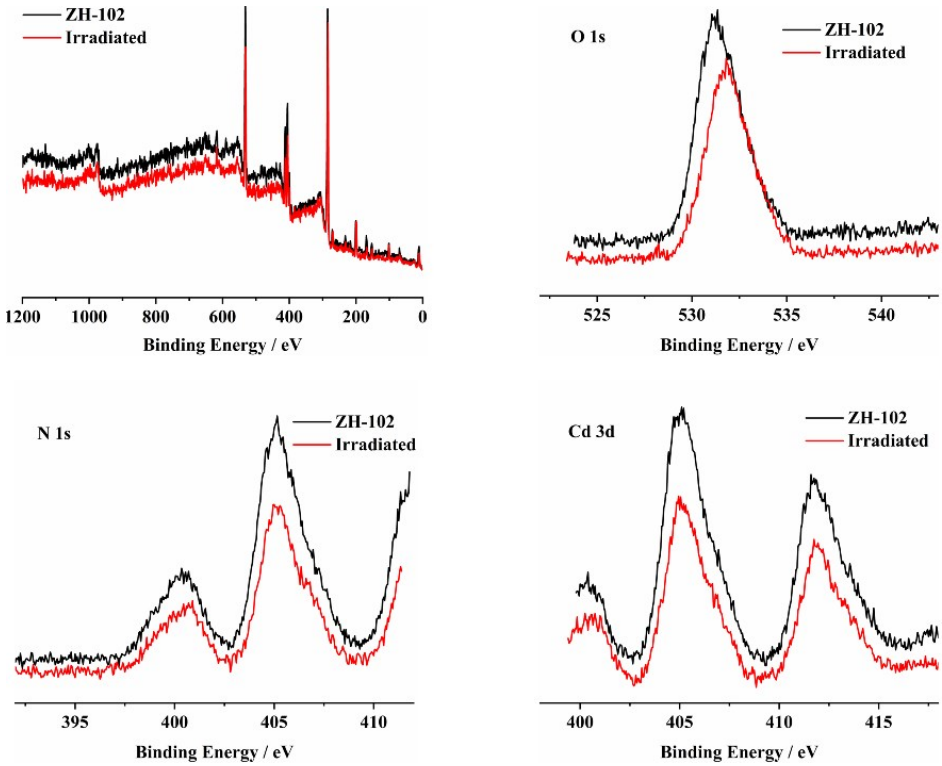


Fig. S9. XPS (Al-Kα) core-level spectra of the **ZH-102** before and after irradiated.

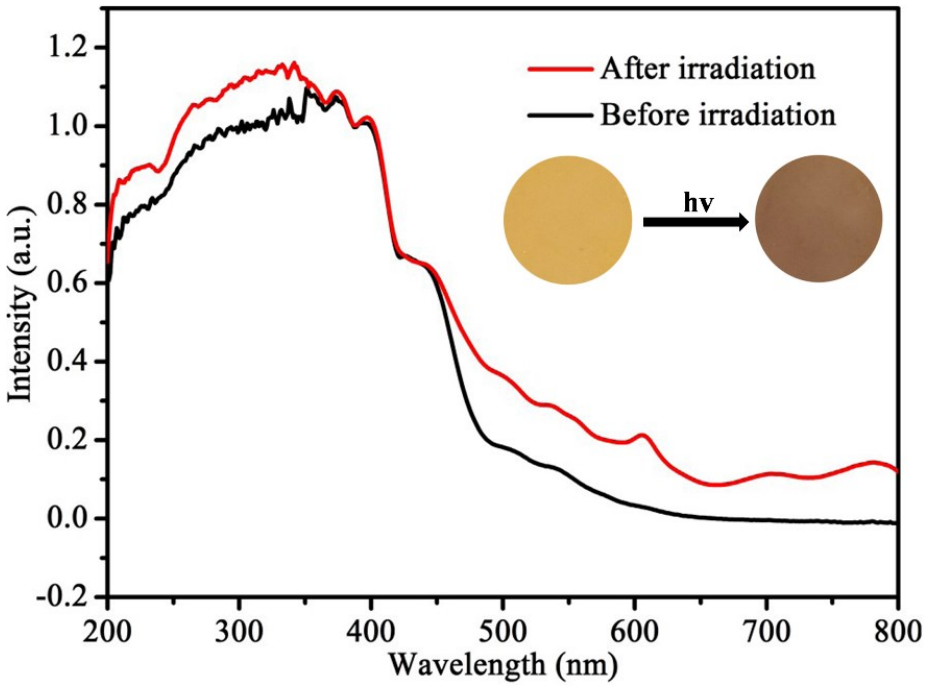


Fig. S10. The UV-Vis spectrum and photographic images of IsoNDI ligand in the photochromic process.

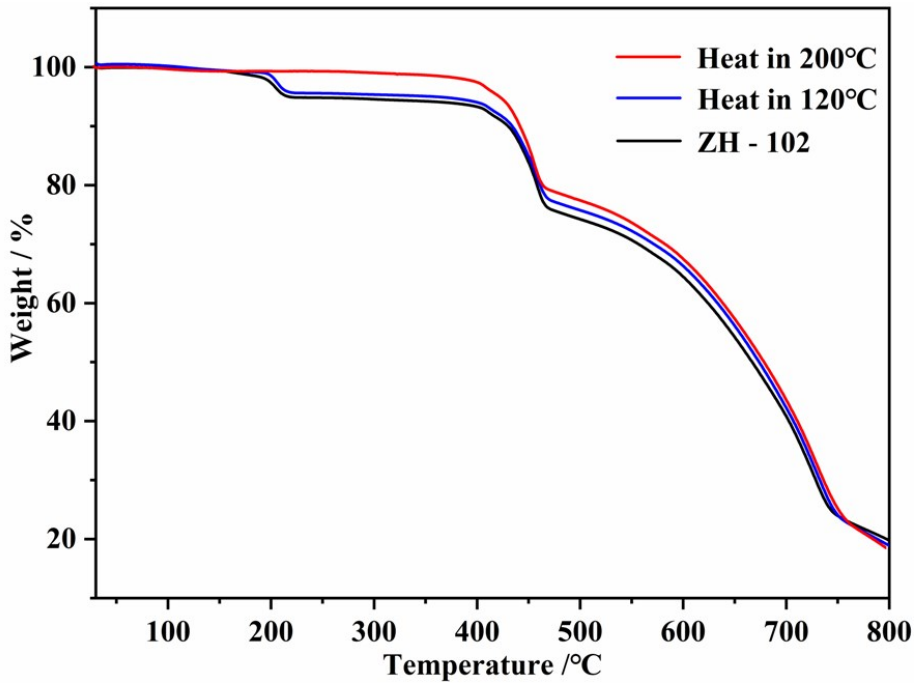


Fig. S11. TG curves of the **ZH-102,** as-synthesized (**ZH-102**), the heated crystals (120 ℃) and the heated crystals (200 ℃).

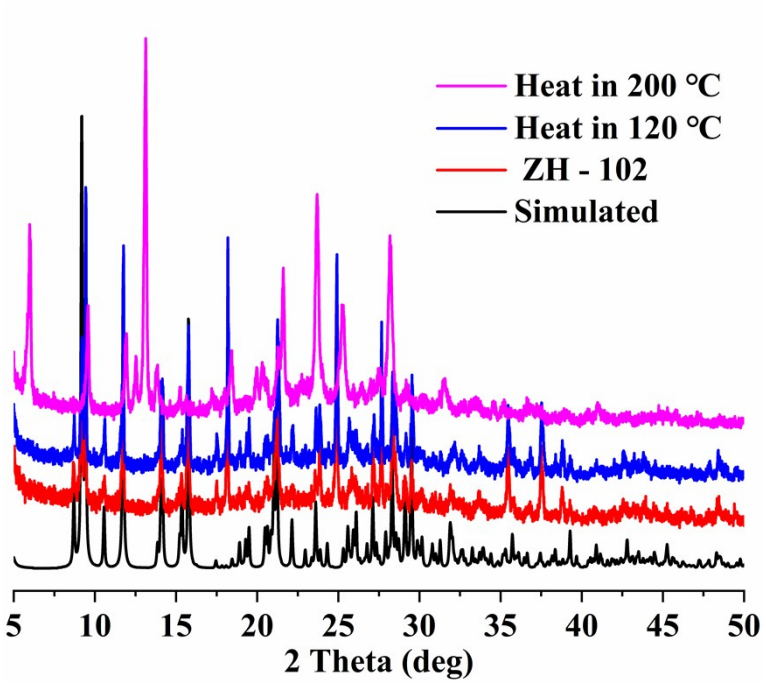


Fig. S12. PXRD patterns of the **ZH-102**; as-synthesized (**ZH-102**), the heated crystals (120 ℃) and the heated crystals (200 ℃).

Table S2. Crystal parameters of complex **ZH-102** after optimization of the structure (VASP) and heating (200 ℃)**.**

	After optimization	**After heating (200 ℃)**
Cryst. Syst	Triclinic	Triclinic
Space group	*P-1*	*P-1*
a (Å)	6.65	6.56
b (Å)	10.78	10.71
c (Å)	19.21	19.01
α (°)	96.43	96.37
β (°)	98.29	98.67
γ (°)	107.41	107.57
V(Å^3)	1285.5	1241

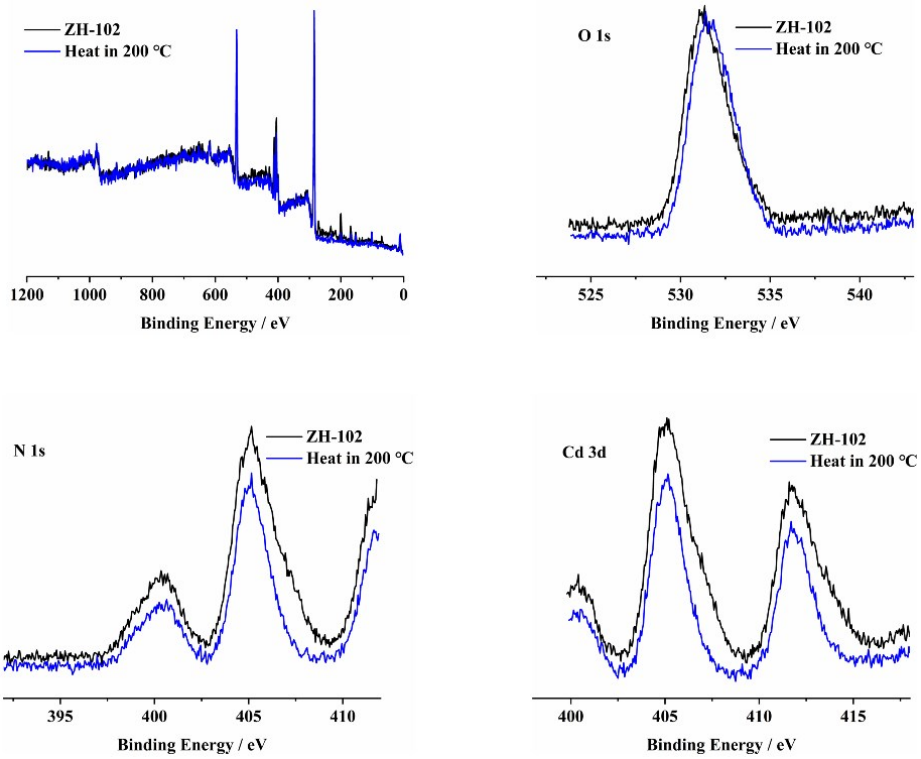


Fig. S13. XPS (Al-Kα) core-level spectra of the **ZH-102** before and after heat in 200 ℃.

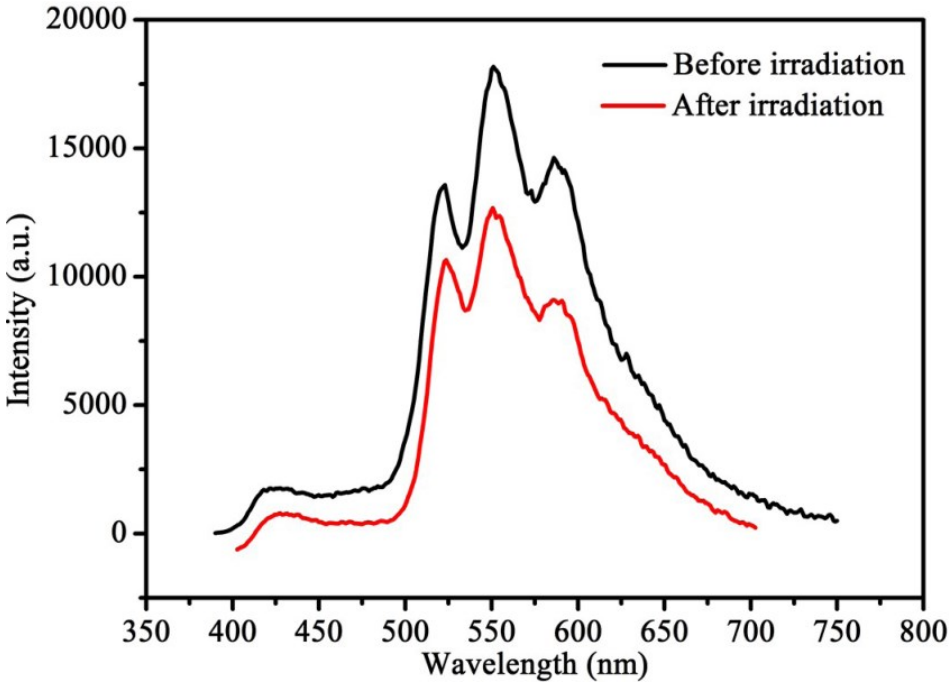


Fig. S14. Photo-controlled luminescence spectrum of IsoNDI ligand.

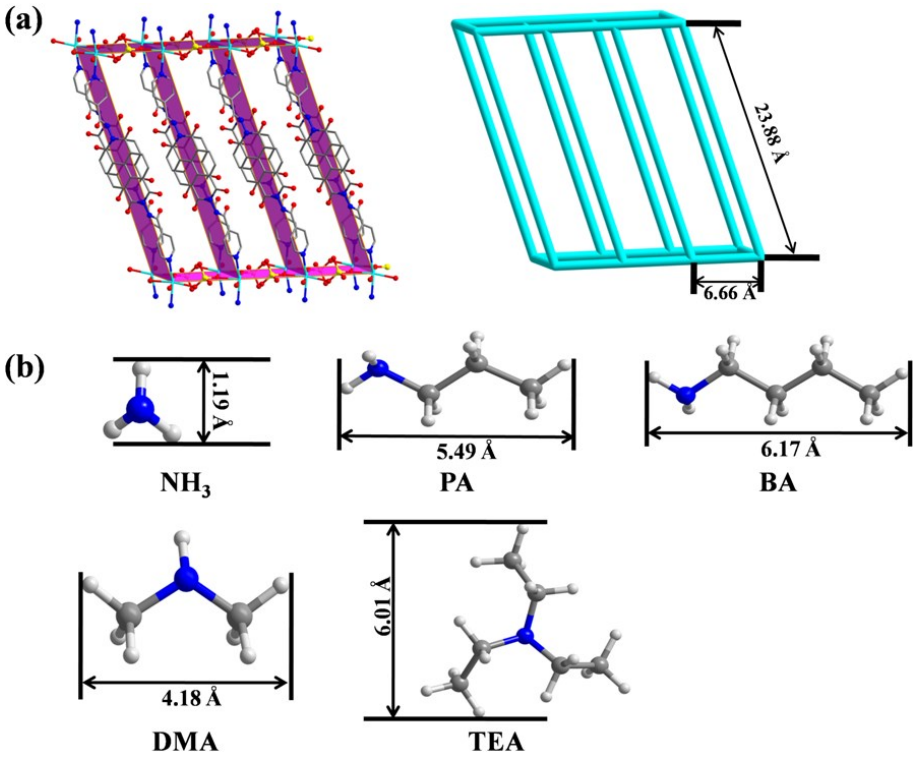


Fig. S15. The rhombic-shaped window-like size of the **ZH-102** and the longest dimension of these five different amines (PA = n-propylamine, BA = n-butylamine, DMA = dimethylamine, TEA = triethylamine).

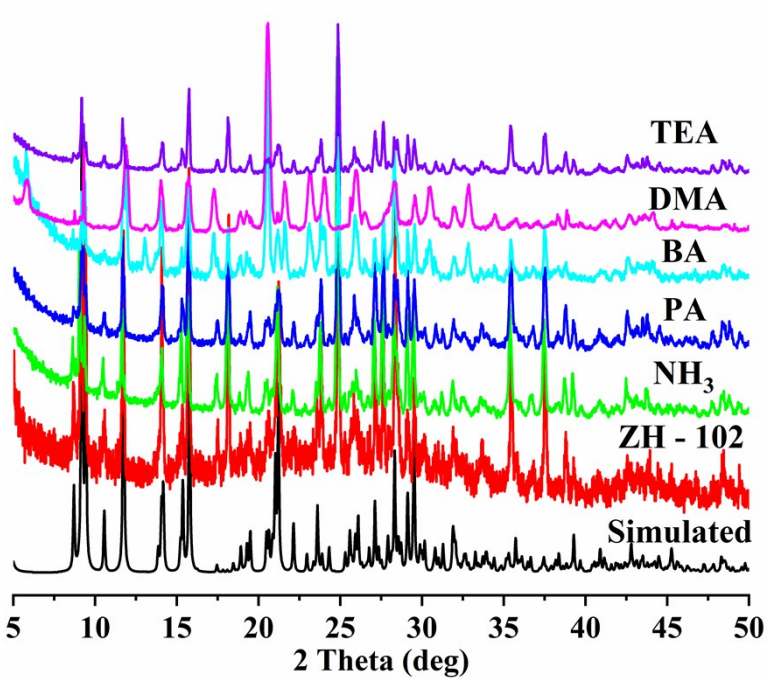


Fig. S16. PXRD patterns of the **ZH-102** and the **ZH-102** after soaking in various amines (PA = n-propylamine, BA = n-butylamine, DMA = dimethylamine, TEA = triethylamine).

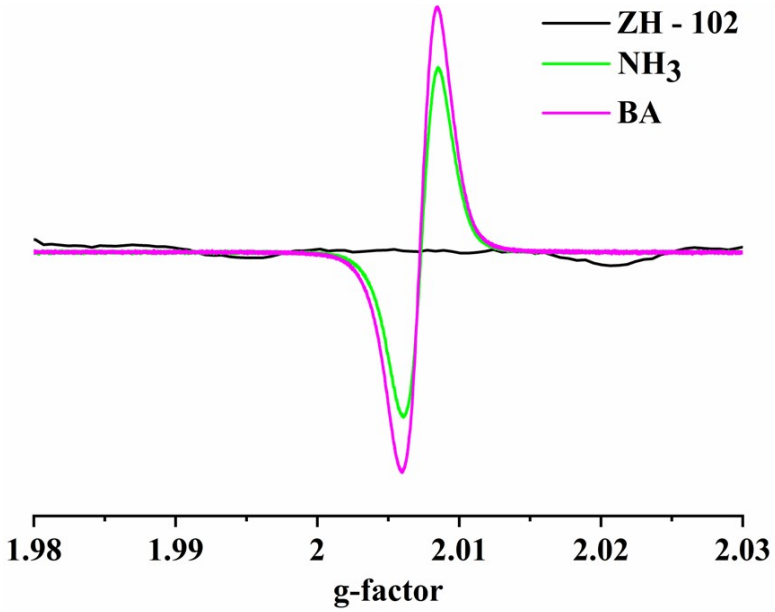


Fig. S17. ESR spectra of the sample of the **ZH-102** before irradiation (black line, **ZH-102**), after the **ZH-102** was exposed to NH_3 and BA.

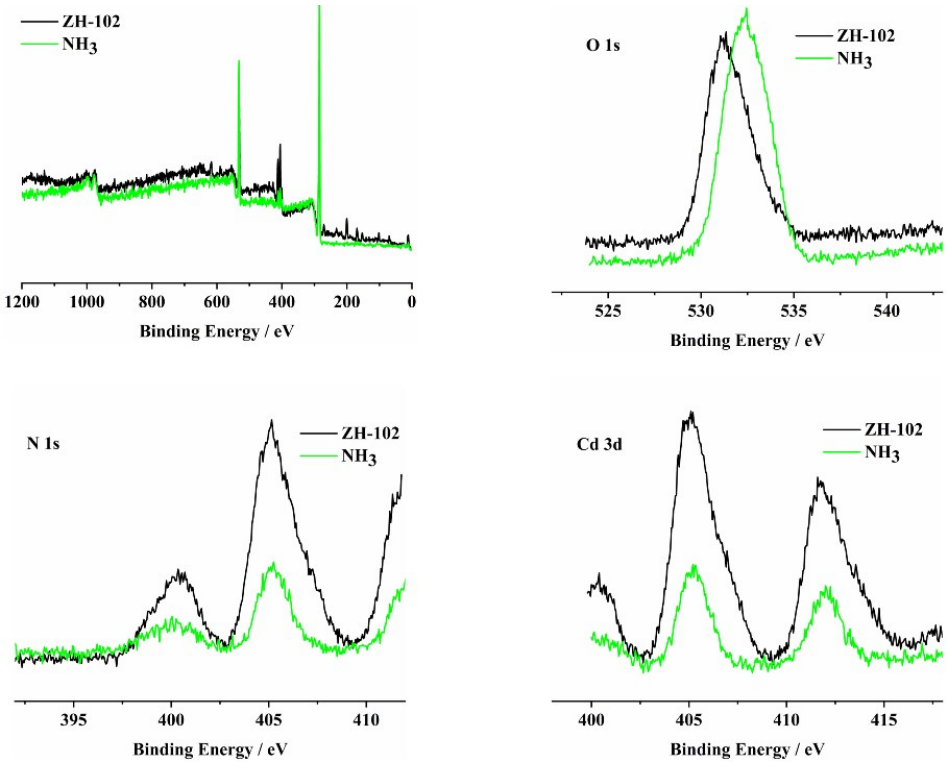


Fig. S18. XPS (Al-Kα) core-level spectra of the **ZH-102** and the **ZH-102** was exposed to NH_3 vapors.

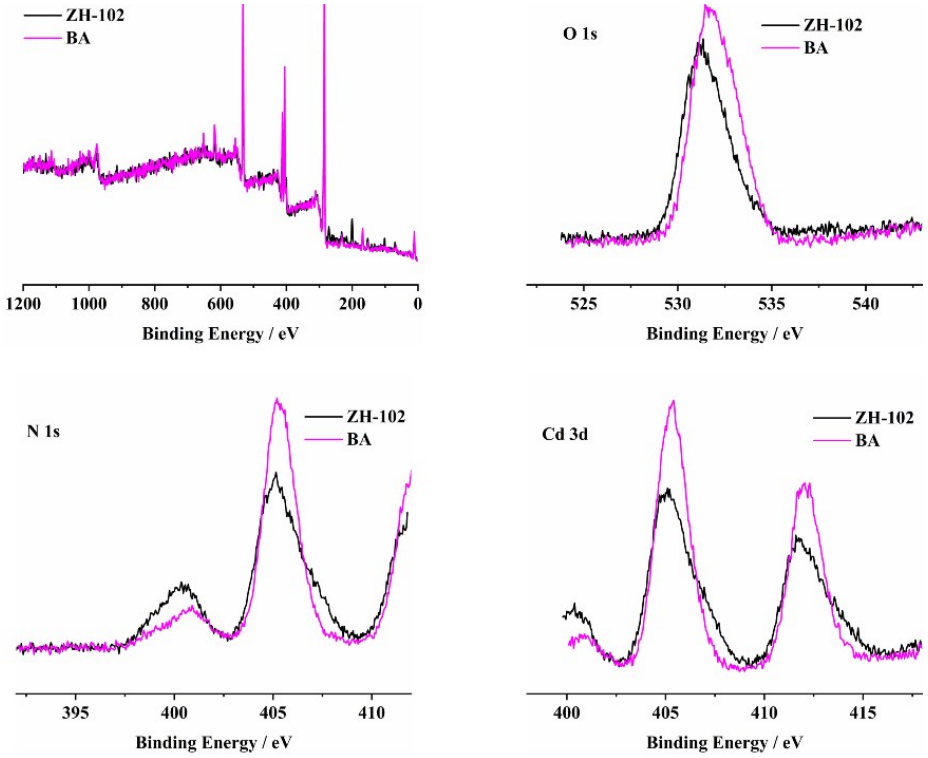


Fig. S19. XPS (Al-Kα) core-level spectra of the **ZH-102** and the **ZH-102** was exposed to n-butylamine (BA) vapors.