Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Ionothermal Synthesis of Photochromic Inorganic-Organic Complex for Colorimetric and Portable UV Index Indication and UVB Detection

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Table S1. Crystal data and structure refinement for NEU-20 [a]

Empirical formula	$C_{40}H_{28}Ga_2N_6O_{20}$
Formula weight	1052.12
Temperature	293 K
Wavelength(Å)	0.71073
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	
a (Å)	26.47(5)
b (Å)	10.667(19)
c (Å)	17.28 (3)
α(deg)	90
β(deg)	125.389(18)
γ (deg)	90
Volume(Å^3)	3976(13)
Z, calculated density(mg m^{-3})	4，1.758
Absorption coefficient(mm^{-1})	1.453
F(000)	2128
Crystal size(mm^3)	0.20 × 0.20× 0.20
θ range(°) for data collection	1.888–27.600
Limiting indices	$-34 \le h \le 34$, $-13 \le k \le 13$, $-22 \le l \le 22$
Reflections collected/unique	17943/4593, [R(int) = 0.1313]
Completeness to θ (%)	25.242, 99.8
Absorption correction	semi-empirical from equivalents
Refinement method	full-matrix least-squares on F^2
Data/restraints/parameters	4593/0/307
Goodness-of-fit on F^2	1.085
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0890$, $wR_2 = 0.2226$
R indices (all data)	$R_1 = 0.1349$, $wR_2 = 0.2599$
Largest diff. peak and hole (eÅ^{-3})	1.406 and -1.147

[a] $R_1 = \sum(\Delta F/\sum(F_o))$, $wR_2 = (\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$ and $w=1/[\sigma^2(F_o^2)+(0.1151P)^2+7.0278P]$ where $P=(F_o^2+2F_c^2)/3$

Table S2. Hydrogen bonds for **NEU20** [A and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1B)...O(7)#1	0.86	2.18	2.880(9)	138.7
N(1)-H(1B)...O(9)#1	0.86	2.11	2.834(10)	141.4
C(1)-H(1A)...O(3)	0.93	2.42	3.348(12)	173.9
C(3)-H(3A)...O(5)#2	0.93	2.46	3.390(11)	174.2
C(6)-H(6A)...O(4)	0.93	2.52	3.158(11)	126.3
C(7)-H(7A)...O(3)	0.93	2.60	3.451(10)	151.5
C(8)-H(8A)...O(5)#2	0.93	2.59	3.456(11)	155.0
C(8)-H(8A)...O(6)#2	0.93	2.47	3.096(10)	124.7
C(9)-H(9A)...O(6)#2	0.93	2.63	3.176(11)	118.3
C(14)-H(14A)...O(7)#2	0.93	2.61	3.503(11)	161.4
C(15)-H(15A)...O(8)#3	0.93	2.54	3.209(11)	129.4

Table S3 Summary of photoresponsive rate in this work compared with literatures

Entry	Sample name	Light suorce	Changed color	k_{obs} (s^{-1})	Ref
1	$[Zn_2(Bpy)(CTA)_4]$	Xe lamp	colorless to purple	1.140×10^{-3}	1
2	$[H_2CPBPY]\cdot[H_2BTEC]$	Xe lamp	pale yellow to green	5.943×10^{-4}	2
3	$[Cd(CPBPY)(m\text{-}BDC)\cdot H_2O$	Xe lamp	yellow to blue	1.2×10^{-3}	3
4	$\{[Zn_3(Cebpy)_2(Hbtc)(H_2btc)_2(OH)_2]\cdot 4H_2O\}_n$	Xe lamp	pale yellow to dark blue	4.29×10^{-3}	4
5	$|C_{10}H_{10}N_2|[GaF(C_2O_4)_2]$	UV light or visible light	colorless to purple	3.86×10^{-3}	5
6	NEU20	UV light	colorless to purple	0.195	This work

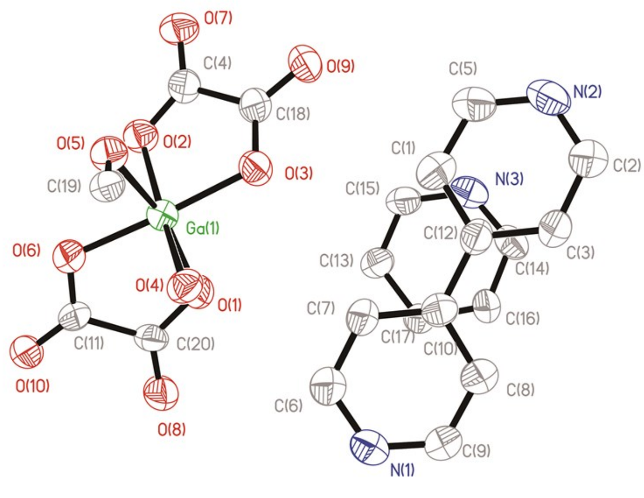

Figure S1. Thermal ellipsoids of NEU20 given at 50% probability, showing the atomic labelling scheme.

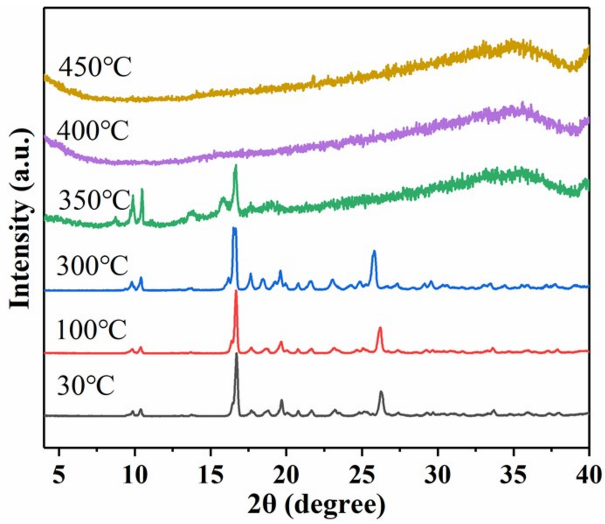

Figure S2. *In-situ* temperature dependent PXRD patterns of **NEU-20** calcined at different temperatures.

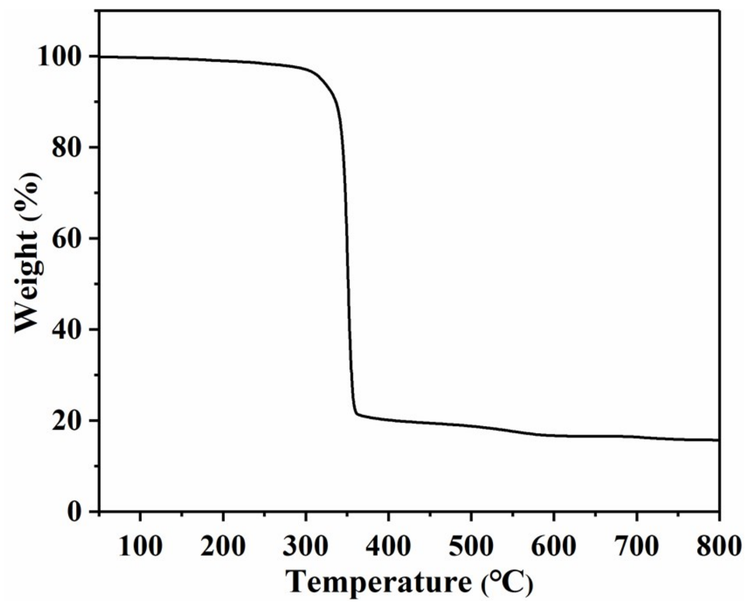

Figure S3. The thermal gravimetric curve of **NEU-20.**

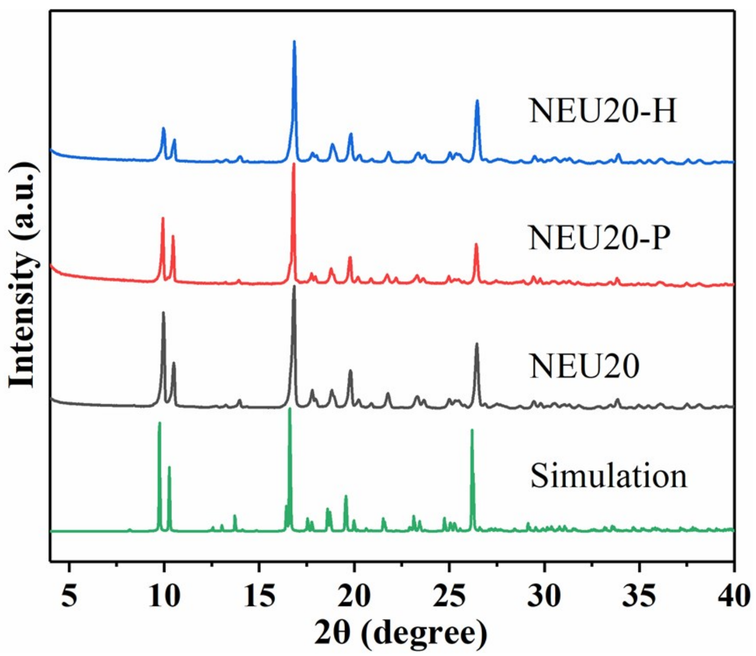

Figure S4. Experimental of **NEU20**, **NEU20-P and NEU20-H** and calculated powder XRD patterns of **NEU20**.

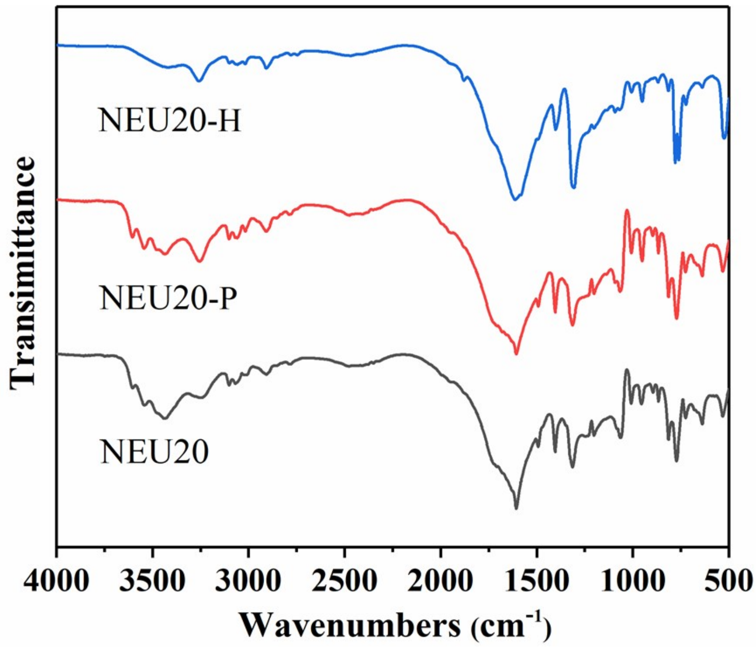

Figure S5. IR curves of **NEU20**, **NEU20-P and NEU20-H**.

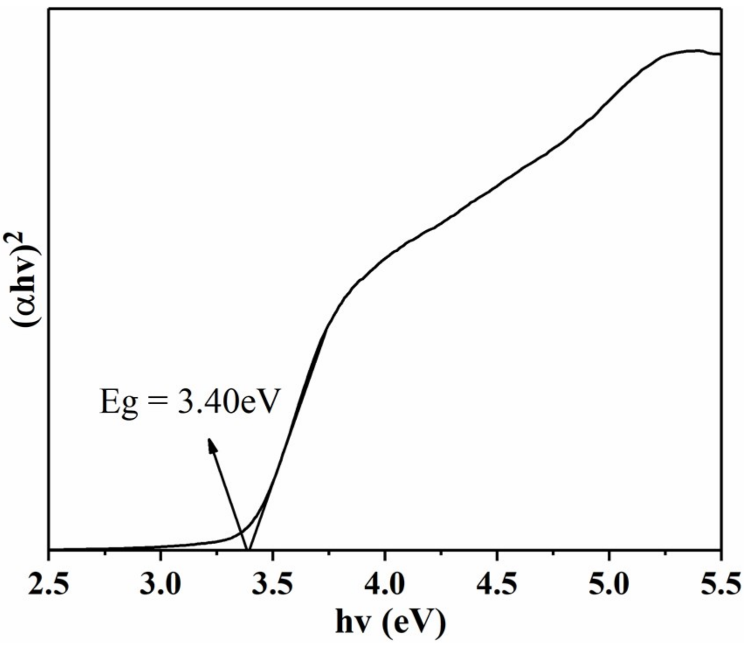

Figure S6. Plot of $(\alpha h\nu)^2$ as a function of hν for the bandgap energy of **NEU20**.

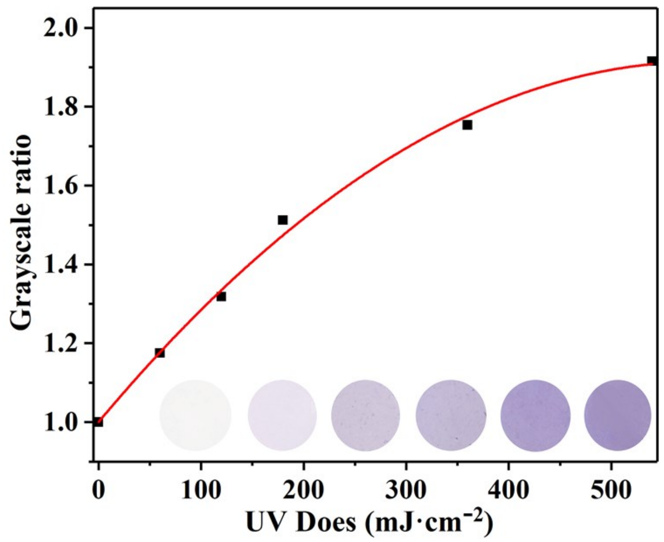

Figure S7. UVA doses detected plot with **NEU20**, following the second-order nonlinear relationship $y=-2.645e^{-6}x^2-0.00311x+1$, $R^2=0.996$.

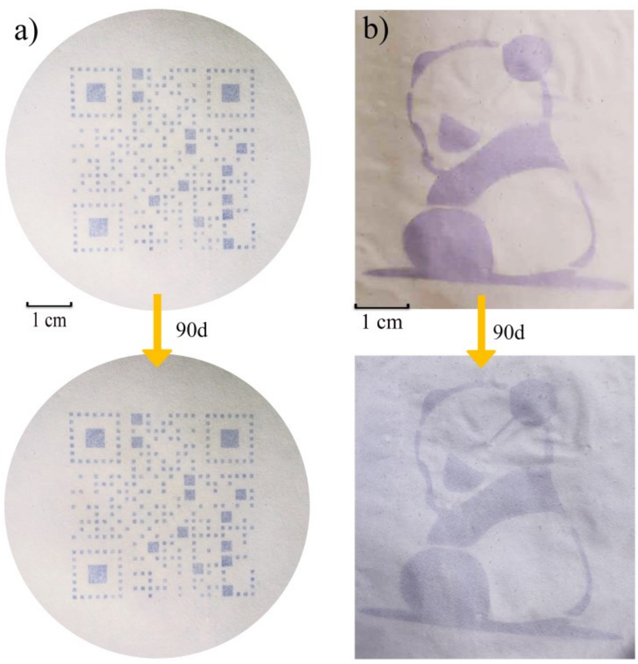

Figure S8. The stability test of a) **NEU20 PAPER** and b) **NEU20/PVDF** under ambient conditions for 90 days.

Table S4 Summary of photochromic performances in this work compared with literatures

Entry	sample name	Light sources	Irradiation intensity	Response time	Color transformation	Bleach condition	Ref
1	$[Zn_2(Bpy)(CTA)_4]$	Xe lamp	300W	-	colorless to purple	130°C for 2h in air.	1
2	$[H_2CPBPY]\cdot[H_2BTEC]$	Xe lamp	150 W	-	pale yellow to green	130°C in air.	2
3	$[Cd(CPBPY)(m\text{-}BDC)\cdot H_2O$	Xe lamp	-	-	yellow to blue	120°C	3
4	$\{[Zn_3(Cebpy)_2(Hbtc)(H_2btc)_2(OH)_2]\cdot 4H_2O\}_n$	Xe lamp	-	10min saturated	pale yellow to dark blue	80°C for 2 hours.	4
5	$\|C_{10}H_{10}N_2\|[GaF(C_2O_4)_2]$	UV light or visible light	48W 300W	10s	colorless to purple	110°C for 30 min.	5
6	$\|C_{12}H_{14}N_2\|[Zn_6(PO_4)_4(HPO_4)(H_2O)_2]$	UV light	-	several hours	colorless to blue	230°C for 1 h in air.	6
7	$[Cd(CEbpy)(m\text{-}BDC)(DMF)]\cdot 2H_2O$	UV light	175W	2min	yellow to darker blue	140°C for 4 ~ 6 h .	7
8	$[Zn(HPO_3)(4,4'\text{-}bipy)_{0.5}]$	Xe lamp	300W	>3min	colorless to pink	145°C for 2 hours in air.	8
9	$[Zn(bcbpy)_{0.5}(pma)_{0.5}(H_2O)]\cdot 3H_2O$	UV light	300W	5s	colorless to blue	50°C for 20 min in air.	9
10	$(MV)Bi_2Cl_8$	UV light	-	-	Yellow to black	130°C in air	10
11	$[Cd_{1.5}(H_2L)_{0.5}(Cl)_3(CH_3OH)]_n$	Xe lamp	300W	a few minutes	pale yellow to blue	120°C for 20 min in air.	11
12	$[Mg_2(1,4\text{-}NDC)_2(H_2O)_2](bpy)(H_2O)_4$	Xe lamp	500W	10min	colourless to blue	60°C for 20 min.	12
13	$[Zn(HCOO)_2(4,4'\text{-}bipy)]$	Xe lamp	300 W	-	pale yellow to olive green	120°C for 2h.	13
14	$Eu_2(m\text{-}BDC)_4(MV)$	Xe lamp or sunlight	-	-	brown to green	-	14
15	TbMOF	Xe lamp	300 W	-	bright yellow to dark green	120°C for 1h in air.	15
16	$(hMV)[Bi(hMV)Cl_5]$	Hg UV lamp	150 W	a few minutes	white to blue	120°C for few minutes.	16
17	[Cd(CPBPY)(o-	UV light	-	-	yellow to gray	exposed to	17

	BDC)$(H_2O)]\cdot H_2O$					pure O_2 or air, return slowly.	
18	$[Zn(L_1)(L_3)_{0.5}]\cdot H_2O$	Xe lamp	250 W	20s	pale yellow to pale green	130 °C for 5 min.	18
19	NTHU-9	X-rays	-	-	orange to slate gray	200°C for 12h in air.	19
20	$[H_2(Bpy)][H_3(Pma)]_2$	Xe lamp	300 W	-	yellow to grayish purple	80 °C for 3 min.	20
21	$[Cd_2(ic)(mc)(4,4'\text{-}bipy)_3]_n\cdot 4nH_2O$	light with λ<460 nm	-	-	yellow to blue	80°C for several hours.	21
22	NEU20	UV light	30W	2s	colorless to purple	140°C for 10 min	This work

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