## **Supplementary Information**

## A Solid AND Logic Stimuli-responsive Material with Bright Nondestructive Performance Designed by Sensitive Cuprophilicity

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Materials and Instruments: All reactants were reagent grade and used as purchased without further purification. Elemental analyses for C, H and N were carried out on a German Elementary Vario EL III instrument. The FT-IR spectra were performed on a Nicolet Magna 750 FT-IR spectrometer using KBr pellets in the range of 4000–400 cm<sup>-1</sup>. Thermogravimetric analyses were recorded on a NETZSCH STA 449C unit at a heating rate of 10 °C·min <sup>-1</sup> under nitrogen atmosphere. The powder X-ray diffraction (XRD) patterns were collected by a Rigaku DMAX2500 X-ray diffractometer using Cu K $\alpha$  radiation ( $\lambda = 0.154$  nm). Luminescent spectra of the compound were measured on an Edinburgh Instruments analyzer model FLS920 with 450W xenon light. The overall luminescent quantum yields of the solid state samples were determined by an absolute method using an integrating sphere (150 mm diameter, BaSO<sub>4</sub> coating) on Edinburgh Instrument FLS920.

Synthesis of  $[CuI(Hdppa)]_{4n} \cdot nH_2O \cdot nC_2H_5OH$  (1): 3-(diphenylphosphino)propanoic acid (Hdppa) (77 mg, 0.3 mmol) and CuI (57 mg, 0.3 mmol) were dissolved in 30 mL solution of H<sub>2</sub>O and C<sub>2</sub>H<sub>5</sub>OH with volume ratio of 1:1. After stirring for about 6 hours at room temperature, the mixture was filtered out, and the filtrate was allowed to evaporate at ambient atmosphere. Colorless crystals of **1** were isolated 5 days later. Yield: 73.16% (0.102 g) based on CuI. Anal. Calcd for C<sub>62</sub>H<sub>68</sub>Cu<sub>4</sub>I<sub>4</sub>O<sub>10</sub>P<sub>4</sub>: C 40.06, H 3.69; found: C 40.15, H 3.62,. Selected IR data (KBr pellet, cm<sup>-1</sup>): 3052s, 2658w, 2580w, 1959w, 1891w, 1810w, 1708vs, 1587vw, 1483m, 1434s, 1252s, 1187m, 1099m, 1027w, 949m, 738s, 693s, 511s.

**Crystal data for compound 1**:  $C_{62}H_{59}Cu_4I_4O_{9.86}P_4$ ,  $M_r = 1847.49$ , triclinic, space group *P*-1, a = 12.7974(16)Å, b = 13.9384(19)Å, c = 22.801(2)Å,  $\Box a = 93.117(4)$ ,  $\Box \beta = 91.872(4)$ ,  $\gamma = 113.996(6)^\circ$ , V = 3703.4(8)Å<sup>3</sup>, Z = 2, T = 113(2) K,  $\rho_{calcd} = 1.657$  g/cm<sup>-3</sup>,  $R_1 = 0.0589$  and  $wR_2 = 0.1488$  for 37185 reflections collected, 9299 observed reflections ( $I > 2\sigma(I)$ ) of 13010 ( $R_{int} = 0.0481$ ) unique reflections and 685 parameters, GooF = 1.058

**X-ray Crystallography:** Structural data of compound **1** were performed on Rigaku-CCD diffractometers equipped with graphite monochromated Mo K $\alpha$  radiation ( $\lambda = 0.71073$  Å) by using the  $\omega$ -scan mode at 113 K. All the structure was refined by full-matrix least-squares fitting on  $F^2$  using the SHELX-97.<sup>1</sup> The coordinate of metal atoms was obtained from the E-map. The

successive Difference Fourier syntheses gave all the coordinates of the non-hydrogen atoms. All non-hydrogen atoms were refined anisotropically except solvent ethanol, and hydrogen atoms of the organic ligands (except those on the undeprotonated carboxylate groups) were generated theoretically onto the specific atoms and refined isotropically with fixed thermal factors. The hydrogen atoms of the solvent H<sub>2</sub>O and those on the normal undeprotonated carboxylate groups were found in the electron density map and refined by riding. The hydrogen atoms on solvent ethanol and splitting group C45O5O6H cannot be generated for their highly disorder. The H<sub>2</sub>O and ethanol molecules in the asymmetry unit of **1** were determined by TG-MS analyses (Figure S4 top) and element analyses as well. A summary of the crystallographic data of **1** are listed in Table S3, and the selected bond lengths and angles are listed in Table S4. More details on the crystallographic data for the structures reported in this paper have been deposited in the Cambridge Crystallographic Data Center with CCDC reference numbers 934722 for compound **1**.



Figure. S1 The asymmetric unit of compound 1. The solvent molecules are omitted for clarity.



Figure. S2 Photographs showing compound **1** on an agate mortar under UV irradiation with black light (365 nm): (a) **1** powder after grinding the right-half with a pestle, (b) the same sample under ambient light, (c) entirely ground powder of **1**, (d) partial reversion to the green luminescence by dropwise addition of ethanol onto the center of the ground powder, (e) powder after treatment with ethanol, and (f) repetition of the green emission by grinding the powder with a pestle.



Figure. S3 The excitation spectra of compound 1 at various states of the AND logic gate.



Figure. S4 The excitation and emission spectra of ligand Hdppa at room temperature.



Figure. S5 Top: the TG-MS of compound 1. The TG curve of complex 1 has one weight loss (3.69%) in the temperature range of 80-140 °C, corresponding to the loss (calculated: 3.70%) of molecules of H<sub>2</sub>O and C<sub>2</sub>H<sub>5</sub>OH. It reaches a plateau until 220 °C before the decomposition reaction takes place. The observed species (m/z: 18 and 46) show flux signals in the MS spectra when the temperature rises, which can be assigned to H<sub>2</sub>O and C<sub>2</sub>H<sub>5</sub>OH, respectively. Bottom: TGA curves for 1 at various states of the AND logic gate: fresh sample (black) loses 3.69% weight corresponding to the loss of a H<sub>2</sub>O and a C<sub>2</sub>H<sub>5</sub>OH (calculated: 3.70%); the sample heated at 100 °C (blue) has no loss until decomposition at 280 °C, as removing all the solvents by heating; the sample ground or heated at 50 °C (red) has one weight loss (0.98%) from 35 °C to 105 °C, corresponding to the loss of a molecular of H<sub>2</sub>O (calculated: 0.99%). Insert: the weight loss from 35 °C to 300 °C.



Figure. S6 Simulated and observed PXRD pattern of compound 1 at various states of the AND logic gate.



Scheme. S1 The corresponding schematic representation of the two-input AND logic gate of 1.

Table S1. Hydrogen bonding distances (Å) and angle (°) data for $1^{a}$				
	D–H	HA	DA	D–H…A
O2–H2O10 <sup>i</sup>	0.948	1.784	2.685	157
07–H704 <sup>i</sup>	0.915	1.936	2.702	140
O10–H10BO8 <sup>i</sup>	0.850	2.026	2.820	155

<sup>*a*</sup> Symmetry codes: (i) -x, 1-y, -z.

Table S2. Equivalent truth table for the "NAND" gate for 1

Input 1 (	C2H5OH)	Input 2 (H2O)	Output 1 ( $\lambda_{max} = 573$ nm)
	1	1	0
	1	0	1
	0	1	1
	0	0	1

Complex	1	
Empirical formula	$C_{62}H_{59}Cu_4I_4O_{9.86}P_4$	
Formula weight	1847.49	
Crystal system	triclinic	
Space group	<i>P</i> -1	
<i>a</i> (Å)	12.7974(16)	
<i>b</i> (Å)	13.9384(19)	
<i>c</i> (Å)	22.801(2)	
$\alpha$ (deg)	93.117(4)	
$\beta$ (deg)	91.872(4)	
$\gamma$ (deg)	113.996(6)	
$V(\text{\AA}^3)$	3703.4(8)	
Ζ	2	
Т(К)	113(2)	
$D_c  (\mathrm{g/cm}^{-3})$	1.657	
$\mu (\mathrm{mm}^{-1})$	2.935	
F (000)	1796	
Parameters	685	
$\theta$ range (deg)	2.0–27.6	
GOF on $F^2$	1.058	
$R_1,^a w R_2^b$ $(I > 2\sigma(I))$	0.0589,0.1488	
$R_1$ , <sup><i>a</i></sup> $wR_2$ <sup><i>b</i></sup> (all data)	0.0827, 0.1687	
Reflns. Collected	37185	
Reflns. Unique (R <sub>int</sub> )	13010 (0.0481)	
${}^{a}R_{1} = \Sigma   F_{o}  -  F_{c}   / \Sigma  F_{o} . {}^{b}wR_{2} = [\Sigma w (F_{o}^{2} - F_{c}^{2})^{2} / \Sigma   F_{o}   / \Sigma   F_{o}  F_$	$\Sigma w (F_o^2)^2 ]^{1/2}.$	

Table S3. Crystallographic data and structure refinement details for 1

Bond lengths (Å)				
I1—Cu1	2.6792 (13)	I2—Cu4	2.6981 (13)	
I1—Cu4	2.7081 (13)	I2—Cu3	2.7148 (13)	
I1—Cu2	2.7123 (14)	Cu1—P1	2.252 (2)	
I4—Cu3	2.6574 (13)	Cu1—Cu4	2.9791 (17)	
I4—Cu2	2.6882 (14)	Cu1—Cu3	3.0036 (16)	
I4—Cu1	2.7545 (13)	Cu3—P3	2.253 (2)	
I3—Cu1	2.6730 (12)	Cu3—Cu2	2.9890 (16)	
I3—Cu4	2.6757 (13)	Cu4—P4	2.251 (2)	
I3—Cu3	2.7130 (12)	Cu2—P2	2.244 (3)	
I2—Cu2	2.6785 (15)			
Angles (°)				
Cu1—I1—Cu4	67.14 (4)	P3—Cu3—I2	114.14 (7)	
Cu1—I1—Cu2	70.37 (4)	I4—Cu3—I2	109.88 (4)	
Cu4—I1—Cu2	69.77 (4)	I3—Cu3—I2	102.78 (4)	
Cu3—I4—Cu2	67.99 (4)	P3—Cu3—Cu2	148.05 (7)	
Cu3—I4—Cu1	67.39 (4)	I4—Cu3—Cu2	56.50 (4)	
Cu2—I4—Cu1	69.60 (4)	I3—Cu3—Cu2	105.44 (4)	
Cu1—I3—Cu4	67.69 (4)	I2—Cu3—Cu2	55.77 (4)	
Cu1—I3—Cu3	67.78 (4)	P3—Cu3—Cu1	142.09 (8)	
Cu4—I3—Cu3	71.54 (4)	I4—Cu3—Cu1	57.84 (3)	
Cu2—I2—Cu4	70.43 (4)	I3—Cu3—Cu1	55.47 (3)	
Cu2—I2—Cu3	67.31 (4)	I2—Cu3—Cu1	102.93 (4)	
Cu4—I2—Cu3	71.18 (4)	Cu2—Cu3—Cu1	62.45 (4)	
P1—Cu1—I3	115.45 (7)	P4—Cu4—I3	116.09 (8)	
P1—Cu1—I1	111.48 (7)	P4—Cu4—I2	114.16 (8)	
I3—Cu1—I1	110.87 (4)	I3—Cu4—I2	104.23 (4)	
P1—Cu1—I4	105.56 (7)	P4—Cu4—I1	105.69 (8)	

## Table S4. Selected bond lengths (Å) and angles (°) for $\mathbf{1}^{a}$

I3—Cu1—I4	108.39 (4)	I3—Cu4—I1	109.90 (4)	
I1—Cu1—I4	104.28 (4)	I2—Cu4—I1	106.41 (4)	
P1—Cu1—Cu4	148.20 (8)	P4—Cu4—Cu1	141.45 (8)	
I3—Cu1—Cu4	56.20 (3)	I3—Cu4—Cu1	56.11 (3)	
I1—Cu1—Cu4	56.89 (3)	I2—Cu4—Cu1	103.99 (4)	
I4—Cu1—Cu4	106.08 (4)	I1—Cu4—Cu1	55.97 (3)	
P1—Cu1—Cu3	142.13 (8)	P2—Cu2—I2	115.01 (10)	
I3—Cu1—Cu3	56.74 (3)	P2—Cu2—I4	111.04 (11)	
I1—Cu1—Cu3	105.15 (4)	I2—Cu2—I4	110.05 (5)	
I4—Cu1—Cu3	54.76 (3)	P2—Cu2—I1	108.11 (9)	
Cu4—Cu1—Cu3	63.54 (4)	I2—Cu2—I1	106.85 (5)	
P3—Cu3—I4	112.91 (7)	I4—Cu2—I1	105.20 (5)	
P3—Cu3—I3	106.44 (7)	P2—Cu2—Cu3	146.98 (9)	
I4—Cu3—I3	110.11 (4)	I2—Cu2—Cu3	56.93 (4)	
I4—Cu2—Cu3	55.51 (3)	I1—Cu2—Cu3	104.71 (4)	
<sup>a</sup> Symmetry codes: (i) -x, 1-y, 1-z				

## Reference

 (a) G. M. Sheldrick, SHELXS97, Program for Crystal Structure Solution (1997) University of Göttingen, Göttigen, Germany; (b) G. M. Sheldrick, SHELXL97, Program for Crystal Structure Refinement, (1997) University of Göttingen, Göttigen, Germany.