

Electronic Supplementary Information (ESI)

Boolean logic tree of molecular self-assembly system based on cobalt oxyhydroxide nanoflakes for three-state logic computation, sensing and imaging of pyrophosphate in living cells and in vivo

Xin Xing Zhang,[#] Qiu Yan Zhu,[#] Jiao Yang Lu, Fu Rui Zhang, Wei Tao Huang,* Xue Zhi Ding, and
Li Qiu Xia

State Key Laboratory of Developmental Biology of Freshwater Fish, College of Life Science, Hunan Normal University, Changsha 410081, P. R. China

*Corresponding author:

E-mail: vthuang@hunnu.edu.cn. Fax: (+86)731-8887-2905; Tel: (+86)731-8887-2905

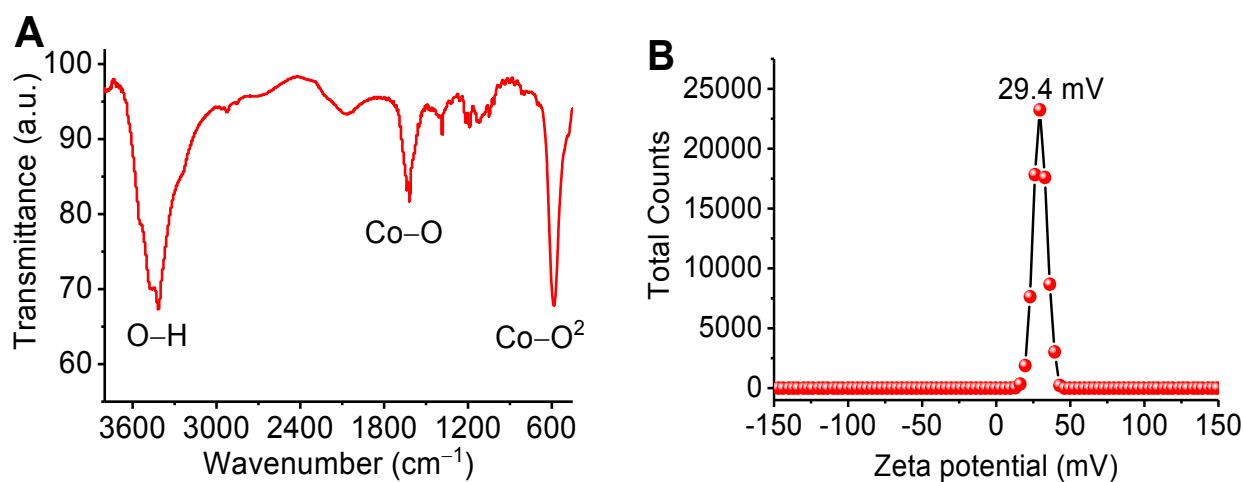


Figure S1. Fourier transform infrared (FT-IR) spectrum (A) and ζ -potential (B) of CoOOH nanoflakes.

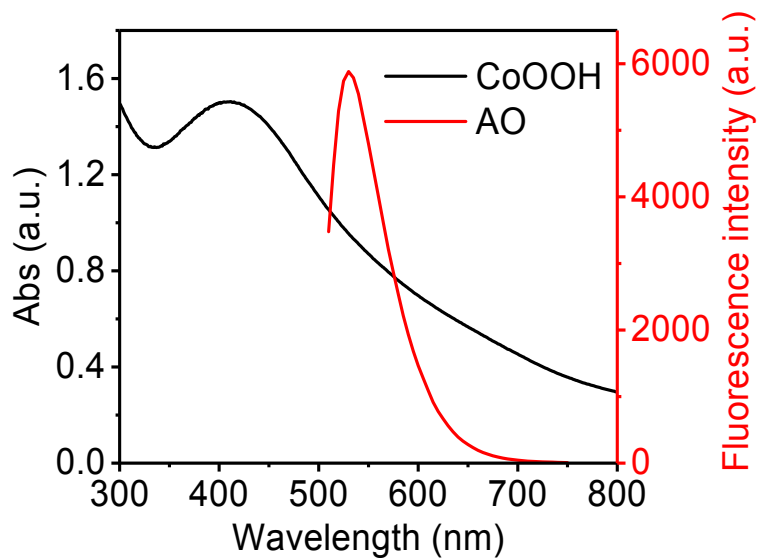
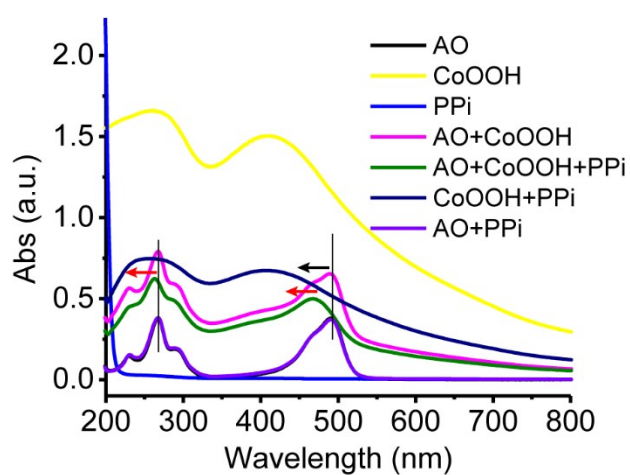


Figure S2. Fluorescence emission spectrum (black line) of AO (10 μM) and the absorption spectrum of the aqueous solution of CoOOH nanoflakes (red line).

Table S1. Comparison of the ζ -potential for AO, PPI, CoOOH, and their mixtures.

	1st measurement	2nd measurement	3rd measurement	ζ -potential
	(mV)	(mV)	(mV)	(mV)
AO	13.3	12.1	12.6	12.7 ± 0.6
PPI	-30.3	-27.8	-21.2	-26.4 ± 4.7
CoOOH	29.4	29	30.4	29.6 ± 0.7
AO-CoOOH-PPI	0.425	0.026	-0.412	0.013 ± 0.4

**Figure S3.** The absorption spectra of AO, CoOOH, PPI, and their mixtures. Arrows indicate the shifts of peaks.

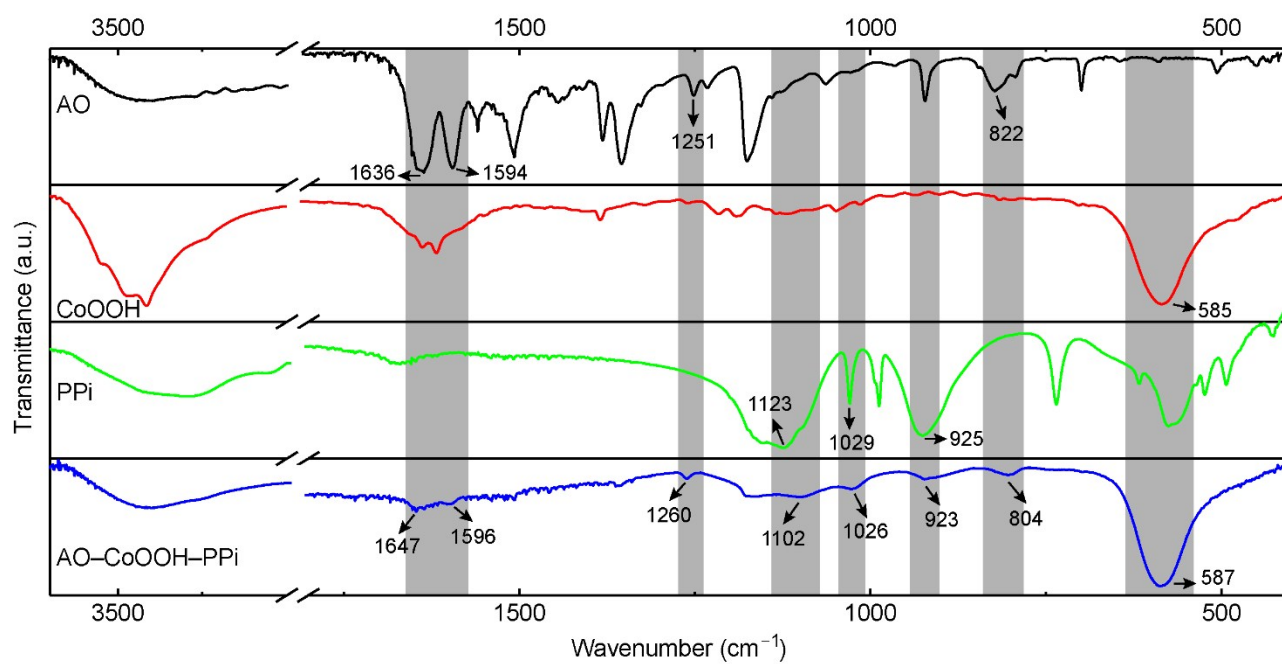


Figure S4. Comparison of FT-IR spectra of AO, PPI, CoOOH, and their mixtures.

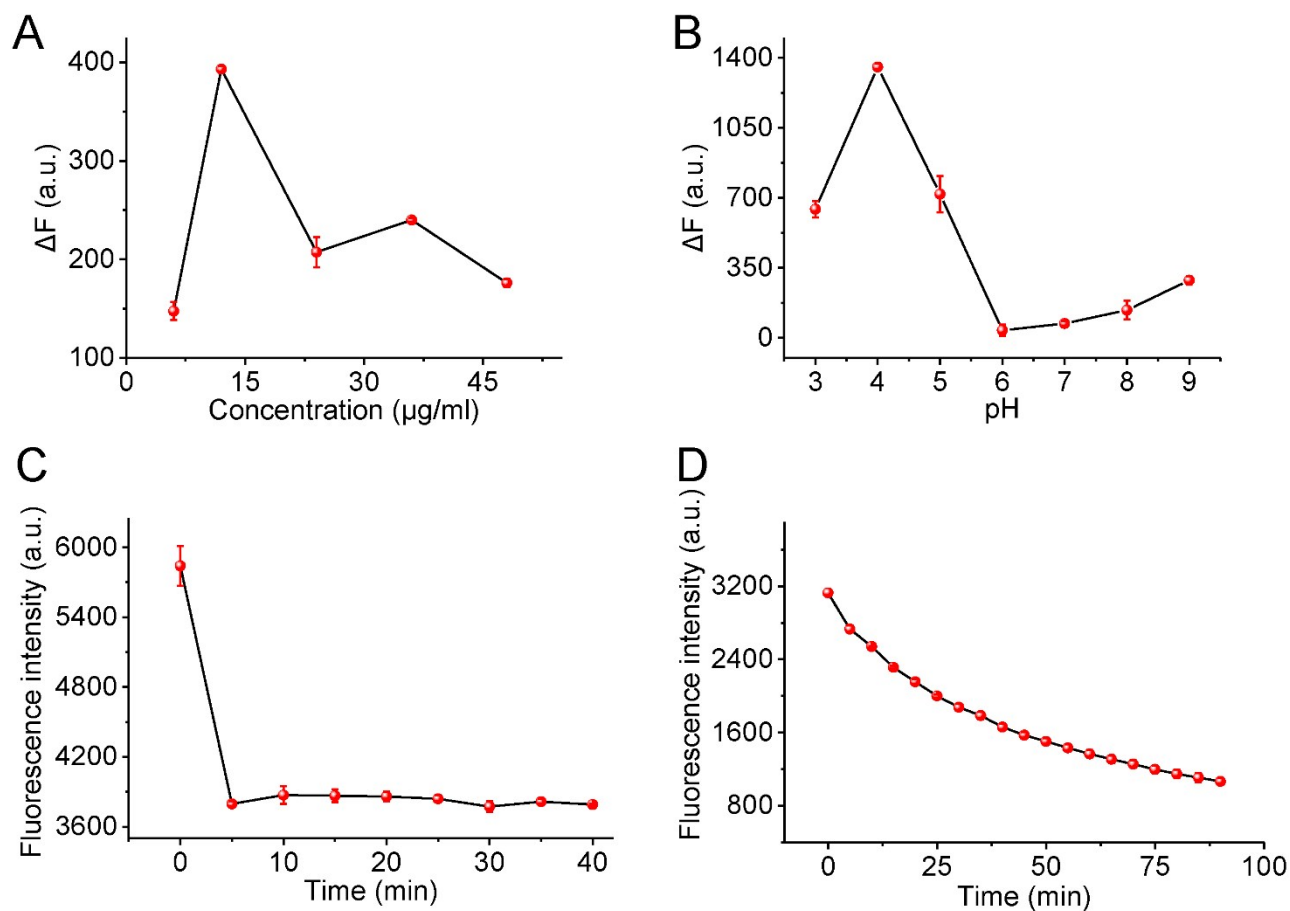


Figure S5. (A) Fluorescence response ($\Delta F = F - F_0$) of different ratio of AO–CoOOH complex to PPI. F and F_0 are fluorescence intensities in the presence and absence of PPI, respectively. (B) Effect of pH on the fluorescence response ($\Delta F = F - F_0$) of AO–CoOOH complex to PPI. pH 4-6: sodium acetate buffer solutions, pH 7-9: Tris-HAc buffer solutions. (C) Time dependence of fluorescence intensity at 530 nm for the AO in the presence of CoOOH. (D) Fluorescence response of AO–CoOOH complex in the presence of PPI as a function of time. (AO 10 μM , CoOOH 6, 12, 24, 36, 48 $\mu\text{g/ml}$, PPI 23.8 μM).

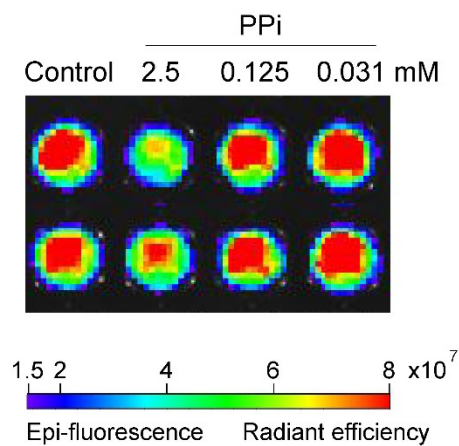


Figure S6. Relative fluorescence intensity of AO-CoOOH complex (1.5 μ M:1.8 μ g/ml) in 96-well plate in different conditions observed by using IVIS Spectrum imaging system. Fluorescent intensity was decreased with increasing concentration of PPI from 0.031 to 2.5 mM. The control represents only AO-CoOOH complex. All measurements were done in sodium acetate buffer (pH 4.0).

Table S2. Comparison of the detection limit and linear ranges of other reported optical PPI assays.

Probe	Detection limit	Linear range	Ref.
Pyridine–biquinoline–metal complexes	850 nM	0–30 μ M	1
Gold nanoparticle-based colorimetric probe	146 nM	No given	2
Gold nanoparticle	No given	130 nM–1.30 mM	3
Gold nanorods	820 nM	5–75 μ M	4
Cysteamine–CdS quantum dots	110 nM	0.11–2.78 μ M	5
Carbon quantum dots	100 nM	0.3–29.7 μ M	6
Carbon dots	500 nM	0.01–1.7 mM	7
DNA-attached magnetic nanoparticles	76 nM	0.2–4 μ M	8
AO–CoOOH complex	20 nM	0.05–6.4 μ M	This work

References

1. Z. Hai, Y. Bao, Q. Miao, X. Yi and G. Liang, *Anal. Chem.*, 2015, **87**, 2678-2684.
2. S. Kim, M. S. Eom, S. K. Kim, S. H. Seo and M. S. Han, *Chem. Commun.*, 2013, **49**, 152-154.
3. J. Deng, P. Yu, L. Yang and L. Mao, *Anal. Chem.*, 2013, **85**, 2516-2522.
4. L. Wang, Q. Song, Q. Liu, D. He and J. Ouyang, *Adv. Funct. Mater.*, 2015, **25**, 7017-7027.
5. T. Noipa, K. Ngamdee, T. Tuntulani and W. Ngeontae, *Spectrochim. Acta A Mol. Biomol. Spectrosc.*, 2014, **118**, 17-23.
6. L. J. Chai, J. Zhou, H. Feng, J. J. Lin and Z. S. Qian, *Sensors Actuators B: Chem.*, 2015, **220**, 138-145.
7. Q. Wang, S. Zhang, H. Ge, G. Tian, N. Cao and Y. Li, *Sensors Actuators B: Chem.*, 2015, **207**, 25-33.
8. L.-l. Tong, Z.-z. Chen, Z.-y. Jiang, M.-m. Sun, L. Li, J. Liu and B. Tang, *Biosens. Bioelectron.*, 2015, **72**, 51-55.