Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Wavelike zinc coordination polymers: anion-modulated ligand conformation and fluorescence detection of 4-aminobenzylamine

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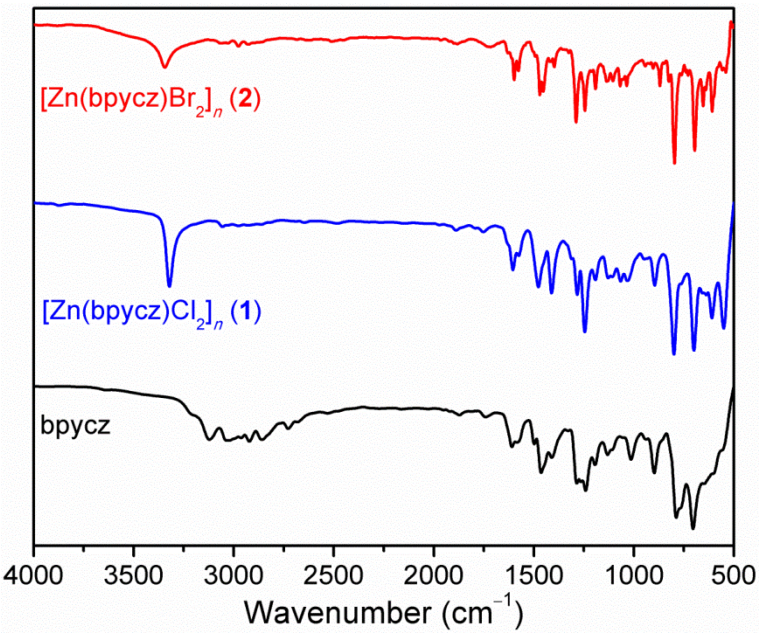


Fig. S1 IR spectra of bpycz and compounds **1** and **2**.

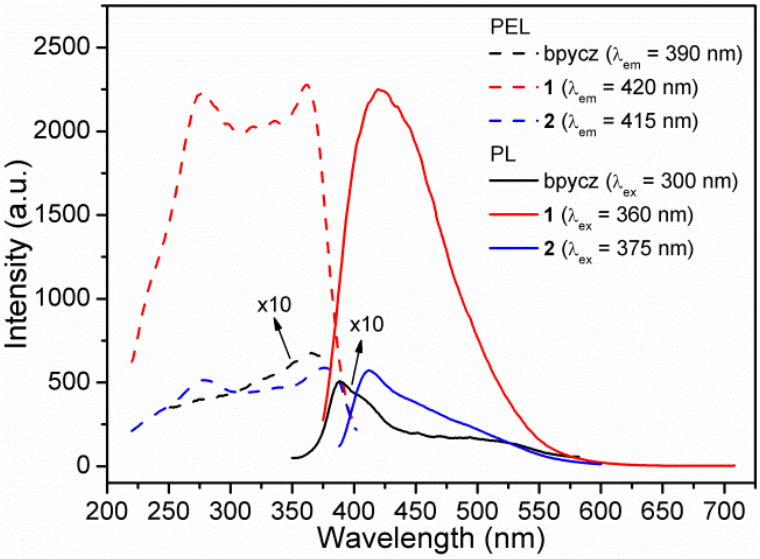


Fig. S2 Solid-state excitation (dashed lines) and emission spectra (solid lines) of bpycz, **1**, and **2**.

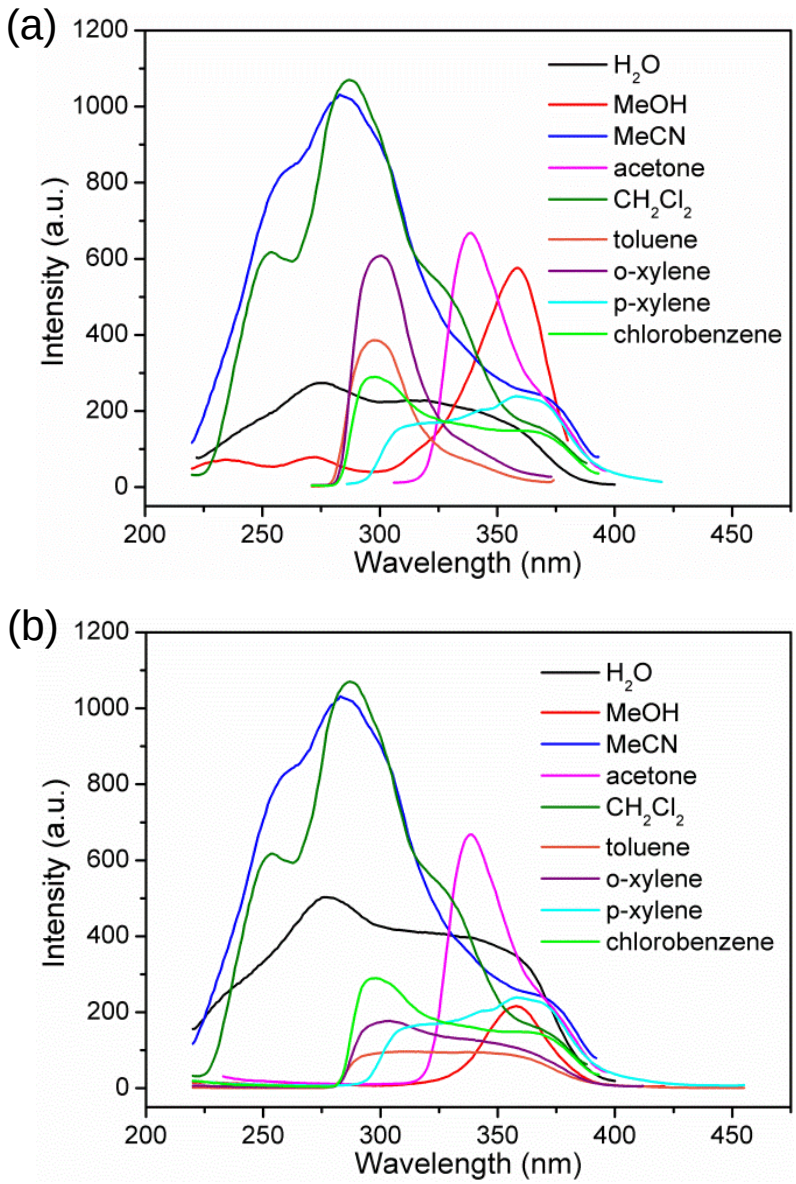


Fig. S3 Excitation spectra of (a) **1** and (b) **2** dispersing in various solvents as suspensions.

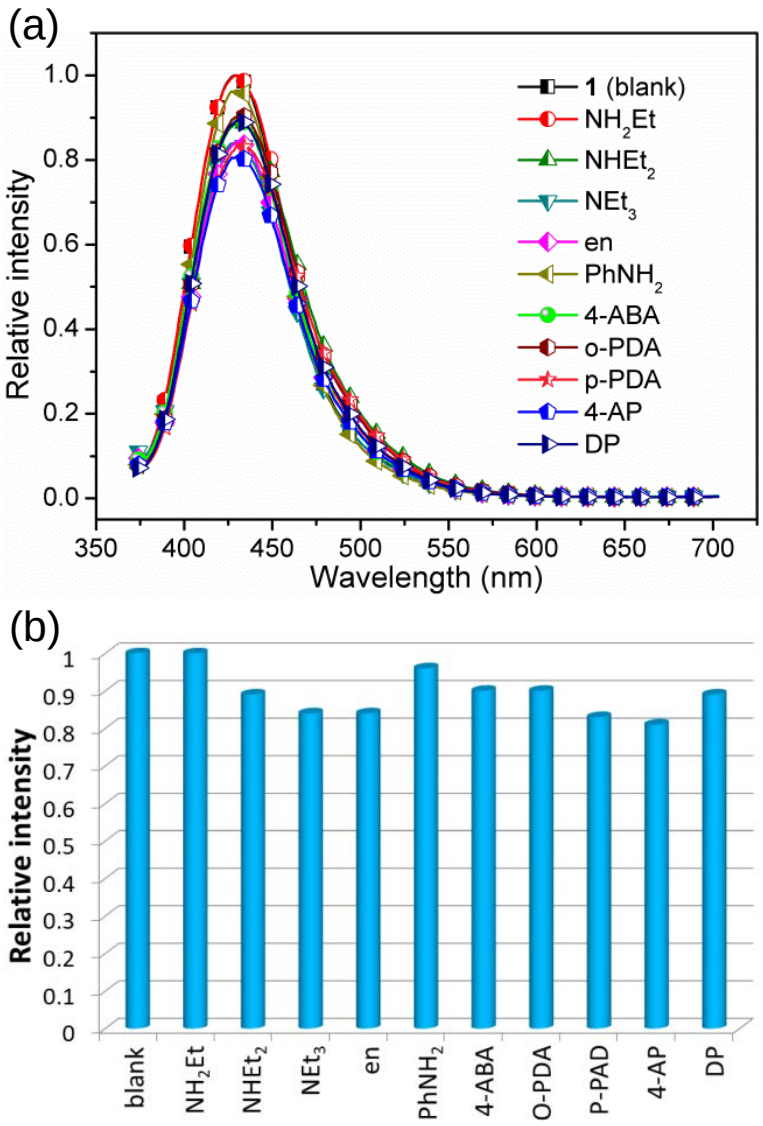


Fig. S4 (a) Fluorescence spectra and (b) relative intensity bar chart of **1** in H_2O suspension before and after addition of 1.0 mM amine analytes upon excitation at 330 nm.

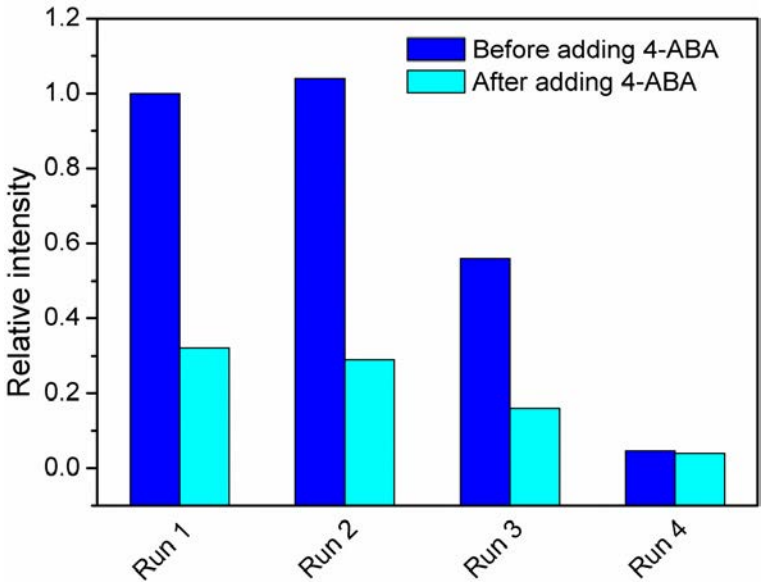


Fig. S5 Relative intensity bar chart of **2** in H_2O suspension before and after addition of 1.0 mM 4-ABA in four sensing–regeneration cycles upon excitation at 330 nm.

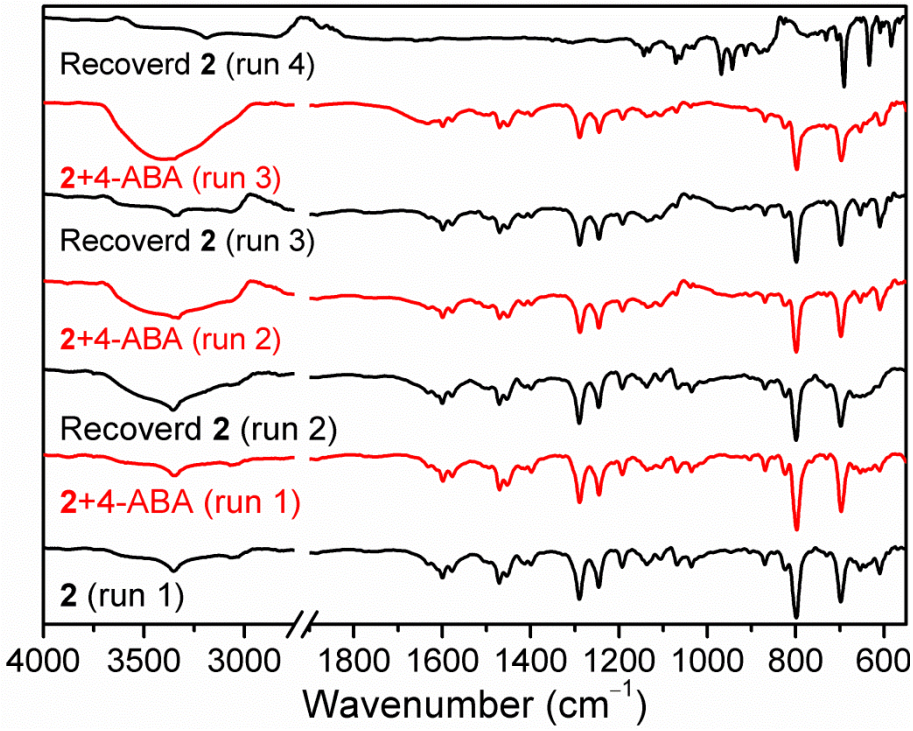


Fig. S6 IR spectra of **2** before and treated with 4-ABA in four sensing–regeneration cycles.

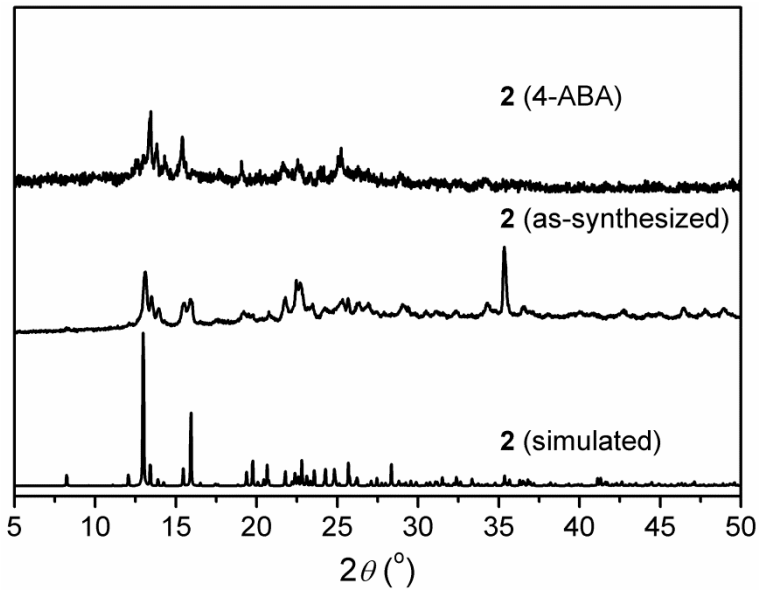


Fig. S7 XRPD patterns of **2**: simulated, as-synthesized, and after treated with 4-ABA for 24 h.

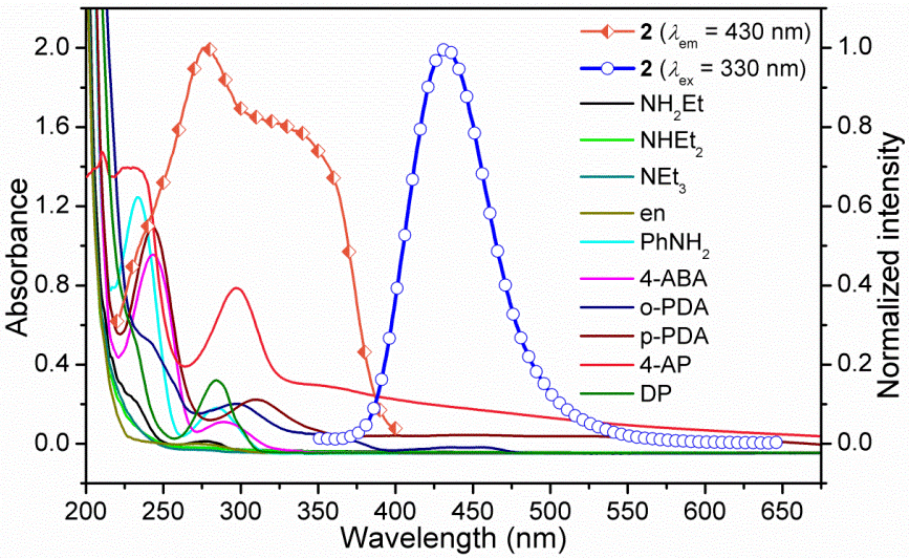


Fig. S8 Overlapped UV/visible absorption spectra of amine analytes in water and the excitation and emission spectra of **2** in H_2O suspension.

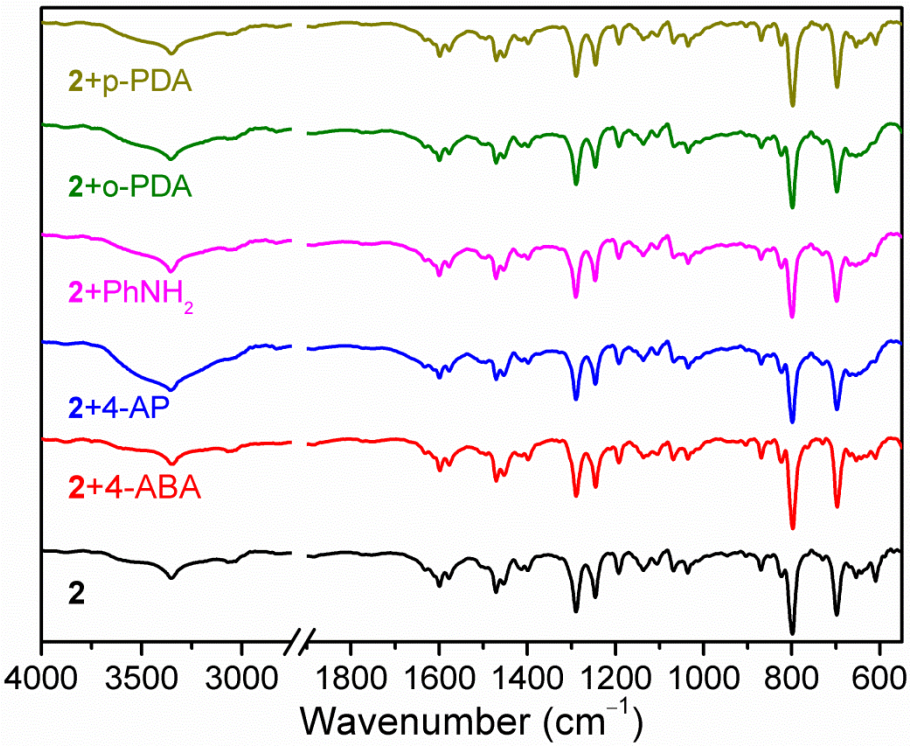
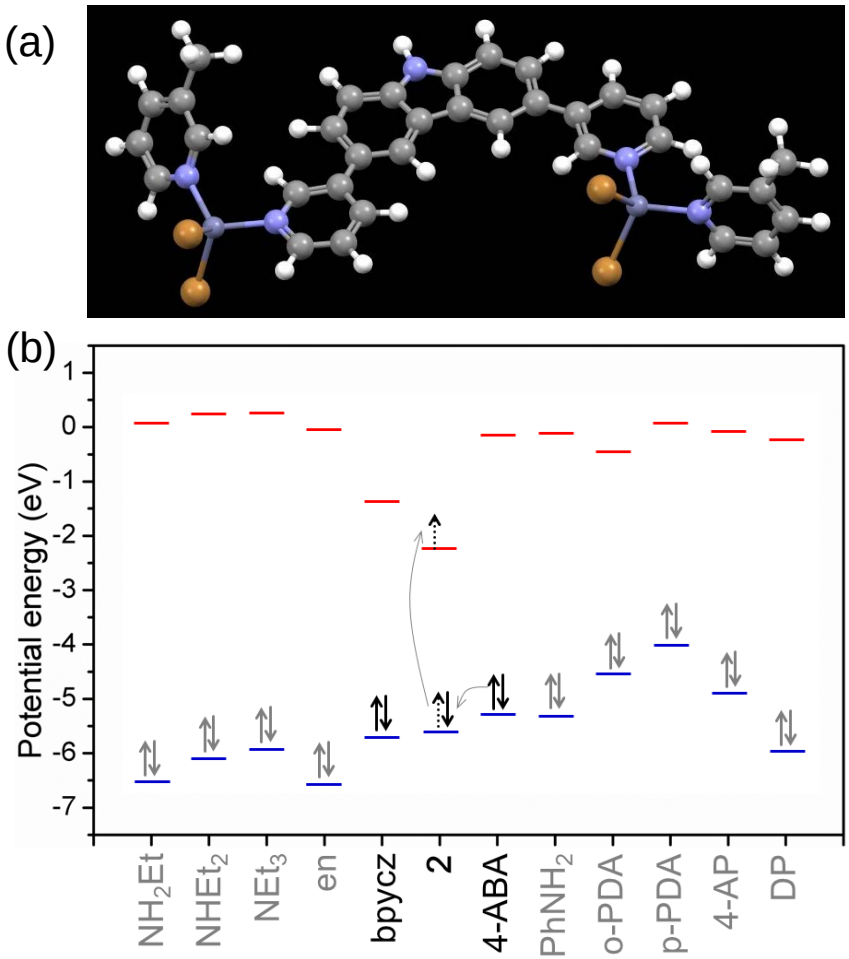


Fig. S9 IR spectra of **2** before and treated with 4-ABA, 4-AP, $PhNH_2$, o-PDA, and p-PDA.



	HOMO (eV)	LUMO (eV)	Energy gap (eV)
bpycz	-5.6763	-1.3720	4.3043
2 (fragment)	-5.5971	-2.2262	3.3709
NH_2Et	-6.5133	0.0732	6.5865
$NHEt_2$	-6.0973	0.2580	6.3553
NEt_3	-5.9166	0.2512	6.1678
en	-6.5291	-0.0503	6.4788
$PhNH_2$	-5.3196	-0.1080	5.2116
4-ABA	-5.2771	-0.1532	5.1239
o-PDA	-4.5160	-0.4522	4.0638
p-PDA	-3.9870	0.0835	4.0705
4-AP	-4.8915	-0.1154	4.7761
DP	-5.9669	-0.2269	5.7400

Fig. S10 (a) The modified partial framework $\{Zn_2Br_4(bpycz)_3(3\text{-}Mepy)_2\}$ used for calculation of the HOMO−LUMO energy levels of **2**. (b) The HOMO−LUMO energy levels of amines, bpycz, and modified partial framework of **2** via the density functional theory at B3LYP/6-31G* level, using Gaussian 09 package of programs.