Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Rational design of a pyrene based luminescent porous supramolecular framework: excimer emission and energy transfer

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Table S1 Selected Bond Distances (Å) for **1**

Cd1-O1	2.321(4)	Cd1-O2	2.355(4)
Cd1-O4	2.220(4)	C12-C13	1.435(11)
Cd1-O1_a	2.321(4)	Cd1-O2_a	2.355(4)
Cd1-O4_a	2.220(4)		

a= 2-x,y,1/2-z

Table S2: Selected bond angles (°) for **1**

O1-Cd1-O2	55.59(13)	O1-Cd1-O4	144.98(12)
O2-Cd1-O4_a	102.12(15)	O1-Cd1-O1_a	84.61(14)
O1-Cd1-O2_a	107.55(14)	O1-Cd1-O4_a	97.47(15)
O2-Cd1-O2_a	159.48(15)	O2-Cd1-O4	91.07(14)
O1_a -Cd1-O4	97.47(15)	O1_a-Cd1-O2	107.55(14)
O2_a-Cd1-O4	102.12(15)		

a= 2-x,y,1/2-z

Table S3: Selected bond distances (Å) for **2**

Zn1-O1	1.973(3)	Zn1-O2	2.501(3)
Zn1-N1	2.093(3)	Zn1-O1_a	1.973(3)
Zn1-O2_a	2.501(3)	Zn1-N1_a	2.093(3)

a= -x,y,1/2-z

Table S4: Selected bond angles (°) for **2**

O1-Zn1-O2	57.28(9)	O1-Zn1-N1	103.94(10)
O1-Zn1-O1_a	138.08(11)	O1-Zn1-O2_a	97.63(10)
O1-Zn1-N1_a	108.18(10)	O2-Zn1-N1	153.44(9)
O1_a-Zn1-O2	97.63(10)	O2-Zn1-O2_a	110.51(10)
O2-Zn1-N1_a	89.21(10)	O1_a-Zn1-N1	108.18(10)
O2_a-Zn1-N1	89.21(10)	N1-Zn1-N1_a	78.81(11)
O1_a-Zn1-O2_a	57.28(9)	O1_a-Zn1-N1_a	103.94(10)
O2_a-Zn1-N1_a	153.44(9)		

a= -x,y,1/2-z

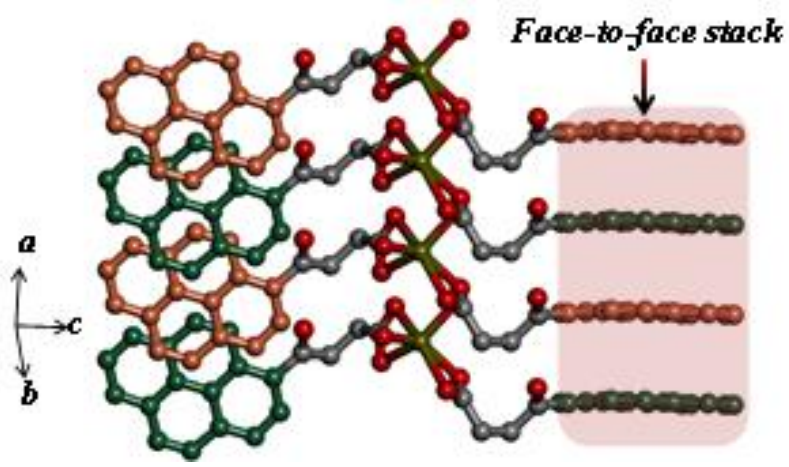

Fig. S1 Off-set face-to-face stacking of molecular complex **1** forming 1D column like structure.

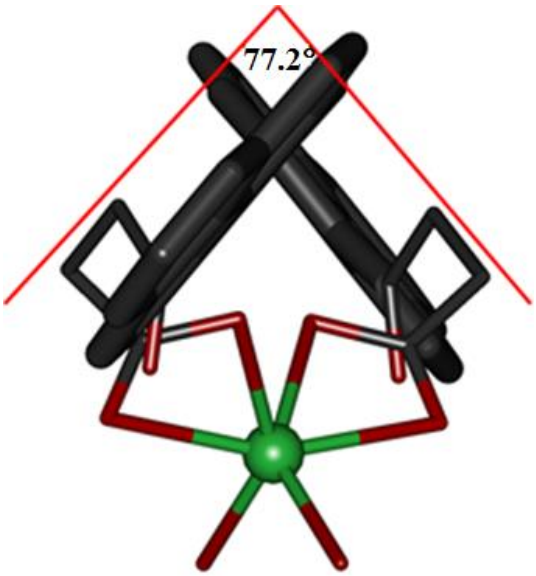

Fig. S2 Dihedral angle between two pyrene rings in **1**.

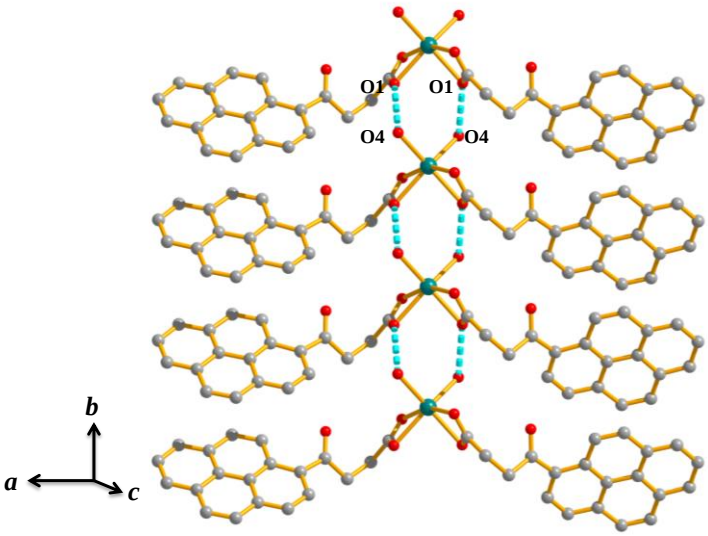

Fig. S3 Hydrogen bonding (cyan dotted lines) between coordinated water molecules and carboxylate oxygens in **1**.

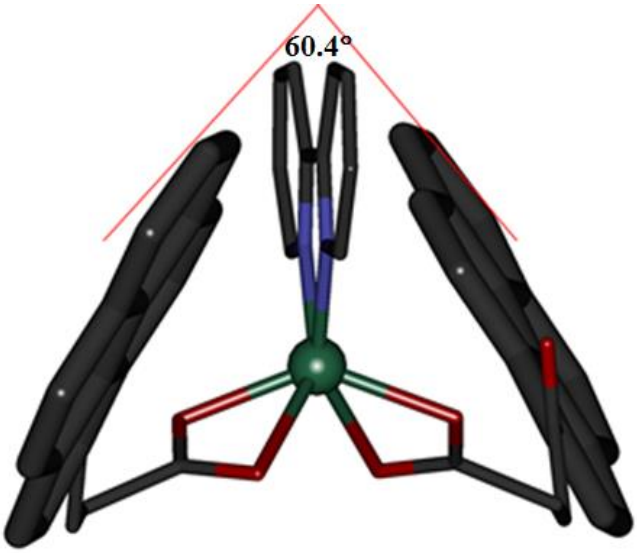

Fig. S4 Dihedral angle between two pyrene rings in **2**.

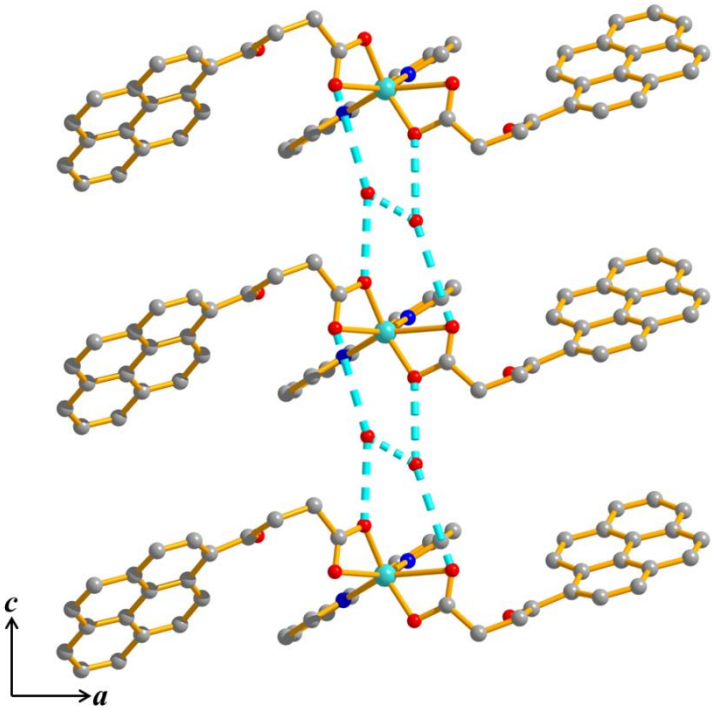

Fig. S5 View of H-bonding interactions among guest water molecules and the carboxylate oxygens in **2**.

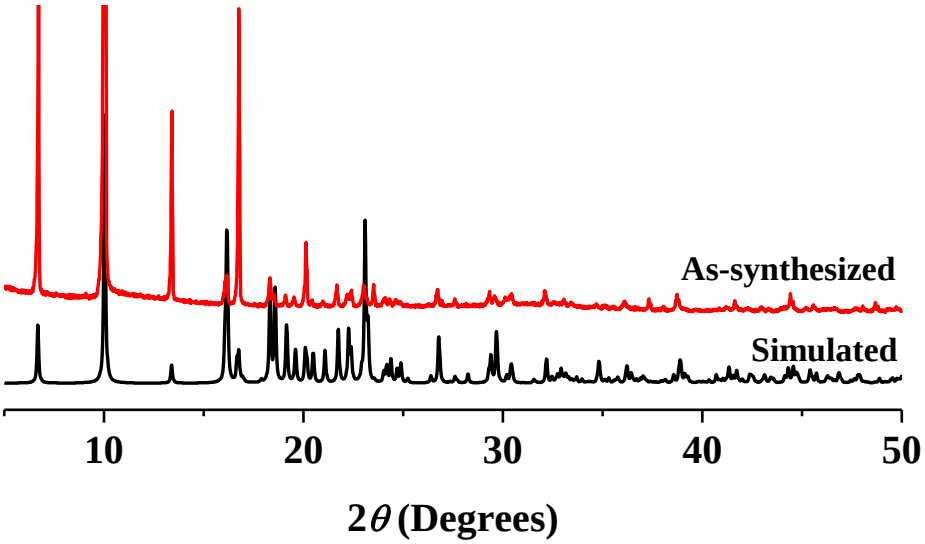

Fig. S6 PXRD patterns of compound **1**: simulated and as-synthesized.

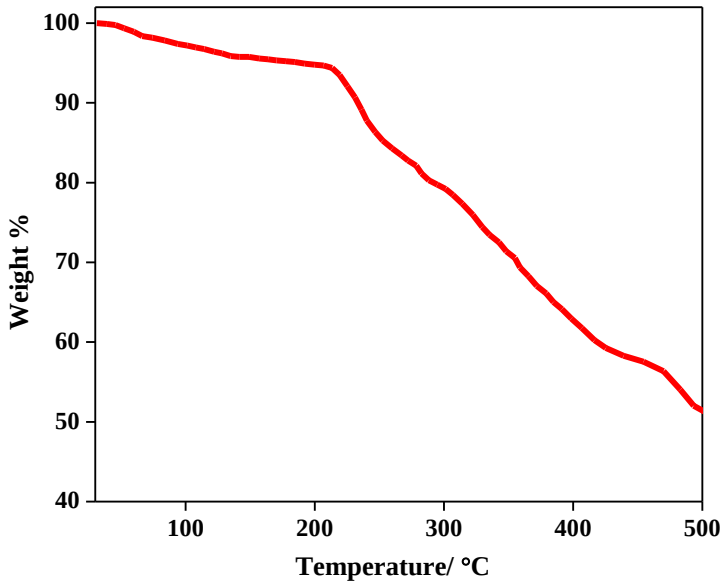

Fig. S7 TG analysis for compound **2** in nitrogen atmosphere (flow rate = 50 mLmin^{-1}) in the temperature range 30–600 °C (heating rate = 5 °C min^{-1}).

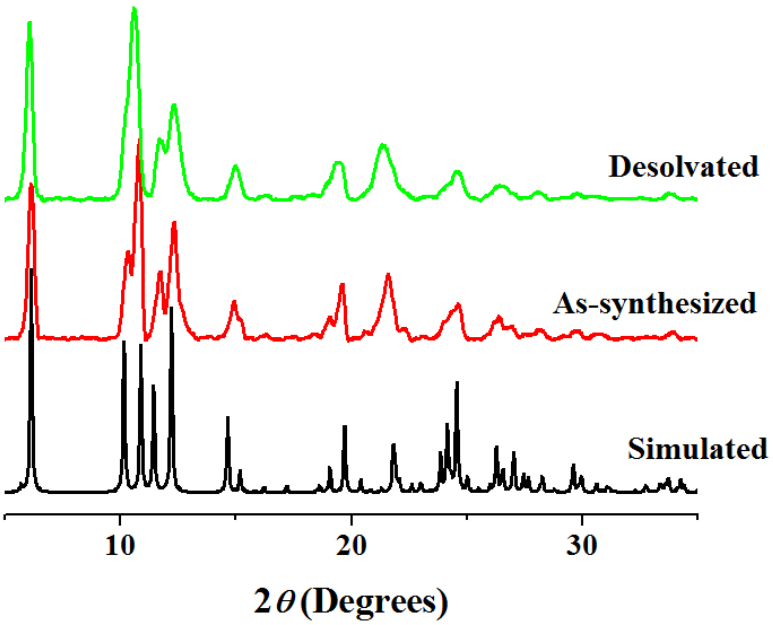

Fig. S8 PXRD patterns of different phases of compound **2**: simulated, as-synthesized and desolvated.

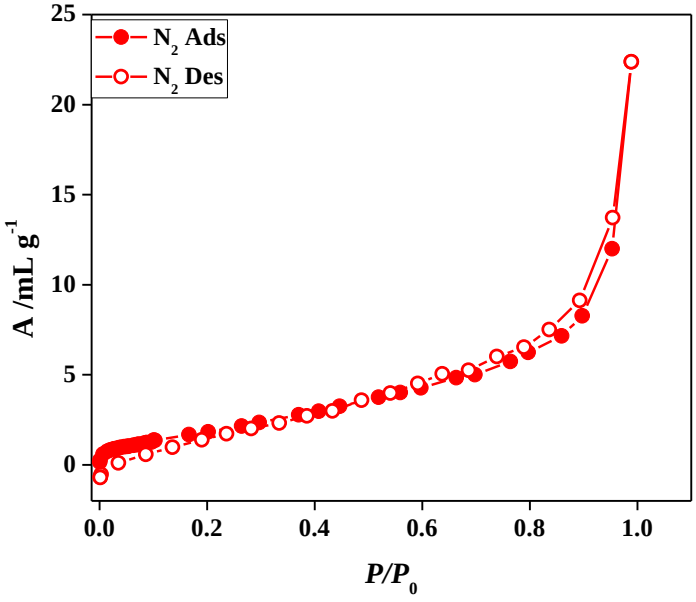

Fig. S9 N_2 adsorption isotherm of **2** at 77 K.

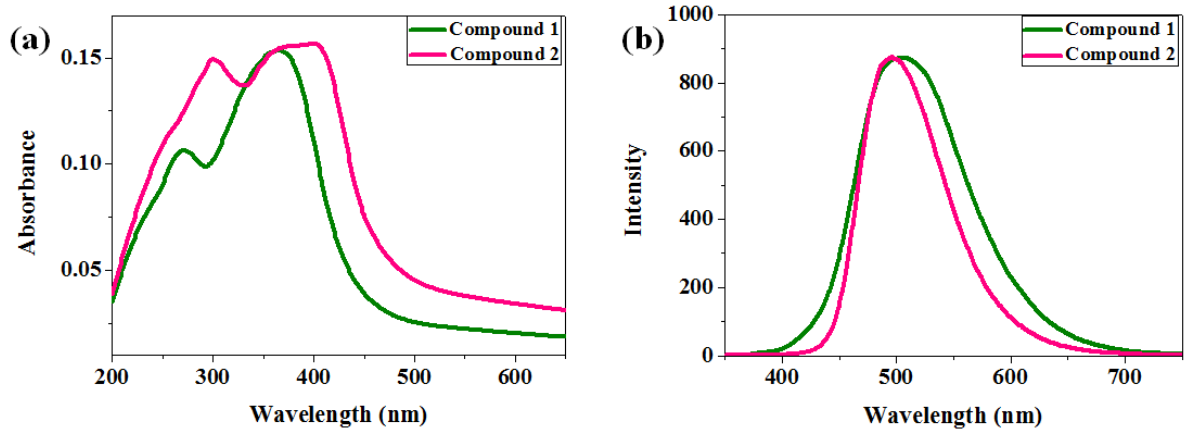

Fig. S10 (a) UV-vis absorption spectra of **1** and **2** in solid state; (b) Emission spectra of **1** and **2** in solid state upon excitation at 330 nm.

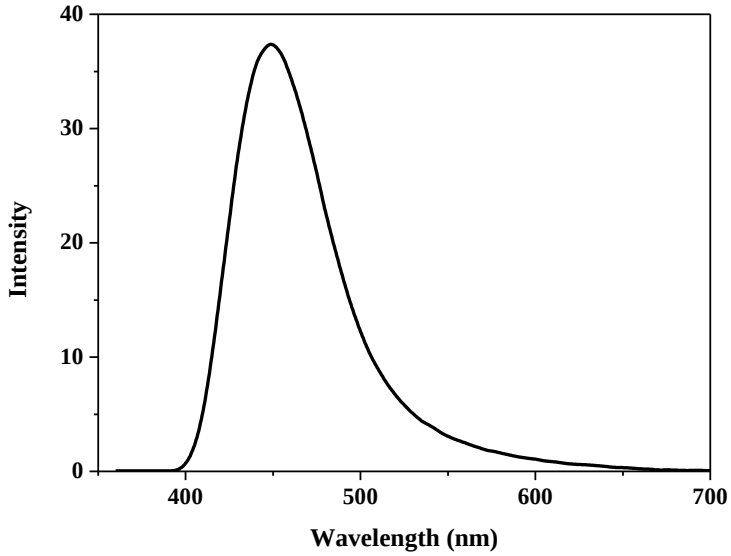

Fig. S11 Emission spectrum of oxo-pba in methanol upon excitation at 330 nm.

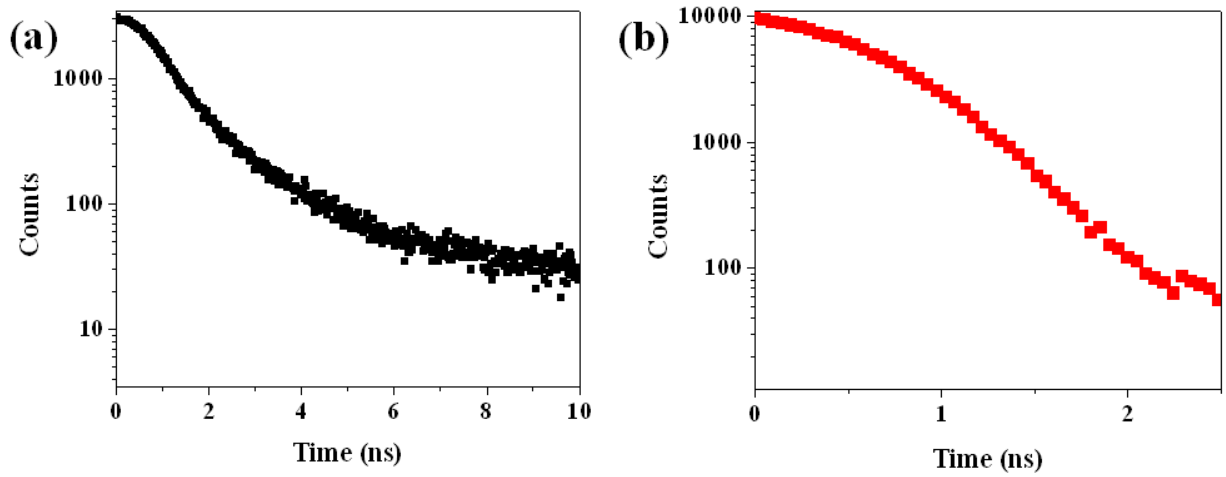

Fig. S12 (a) Fluorescence life time spectrum of oxo-pba dissolved in methanol monitored at 442 nm upon excitation at 270 nm; (b) showing IRF (Instrument Response Function) upon excitation at 270 nm.

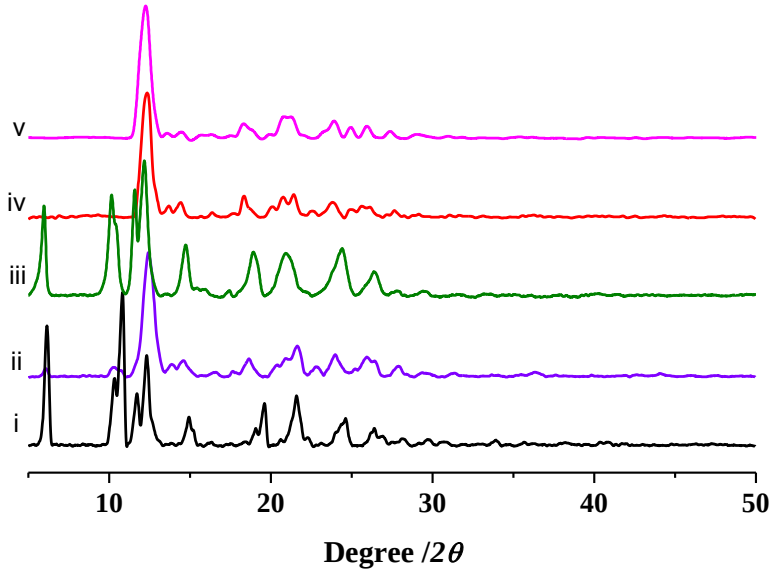

Fig. S13 PXRD patterns of (i) desolvated **2**; (ii) methanol exchanged **2**; (iii) desolvated **2** (heated at 80 ºC) after methanol exchange; (iv) **AO@2** with methanol; (v) **AO@2** heated at 60° C.

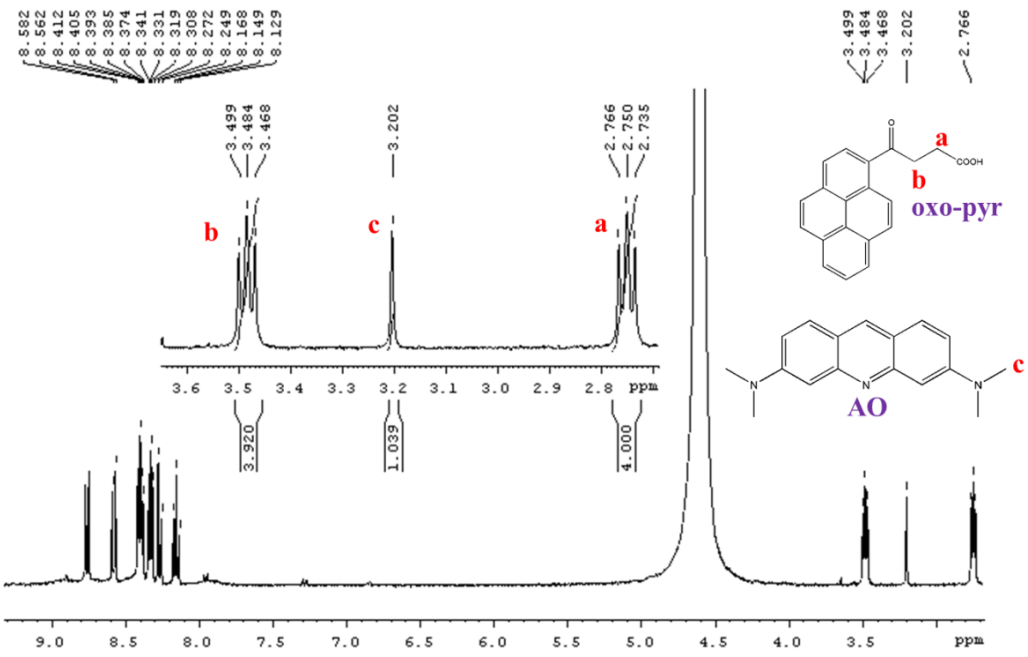

Fig. S14 ^{1}H-NMR spectrum of **AO@2** in DMSO after dissolution in DCl.

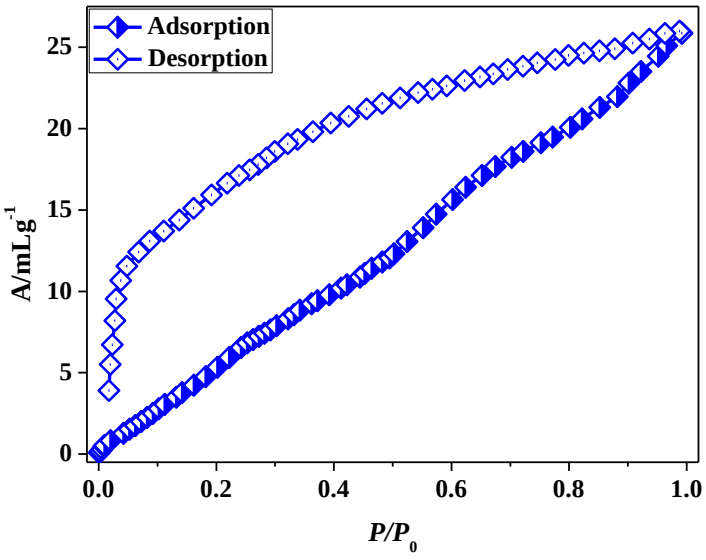

Fig. S15 CO_2 adsorption isotherm of physical mixture of **2** and AO at 195 K.

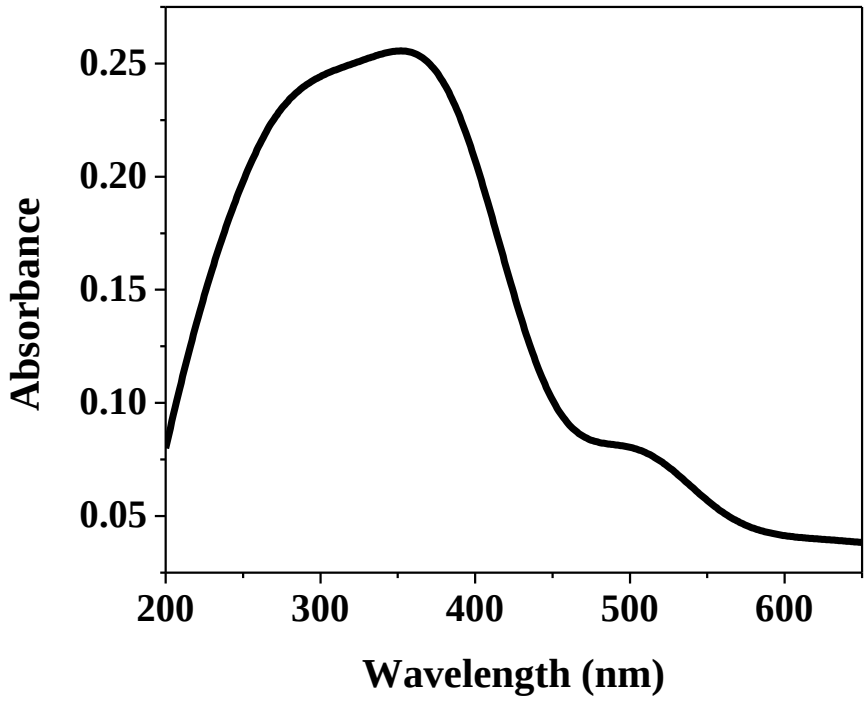

Fig. S16 UV-vis absorption spectrum of **AO@2** in solid state.

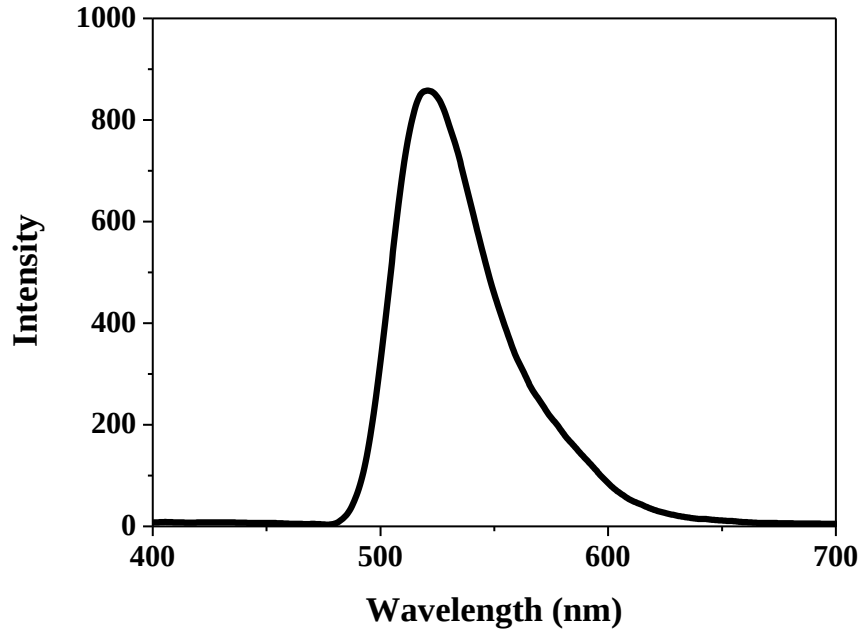

Fig. S17 Emission spectrum of acridine orange in methanol upon excitation at 300 nm.

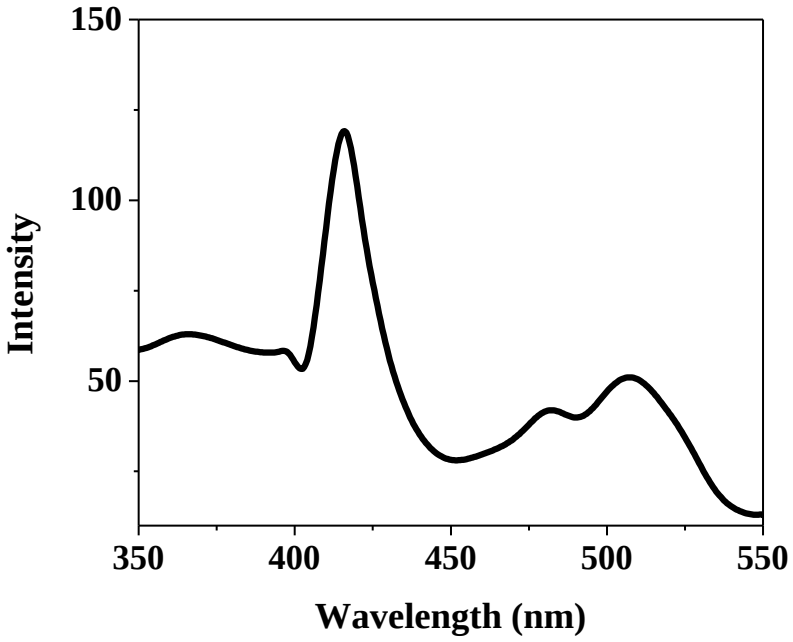

Fig. S18 Excitation spectrum of **2@AO** observed at 575 nm.

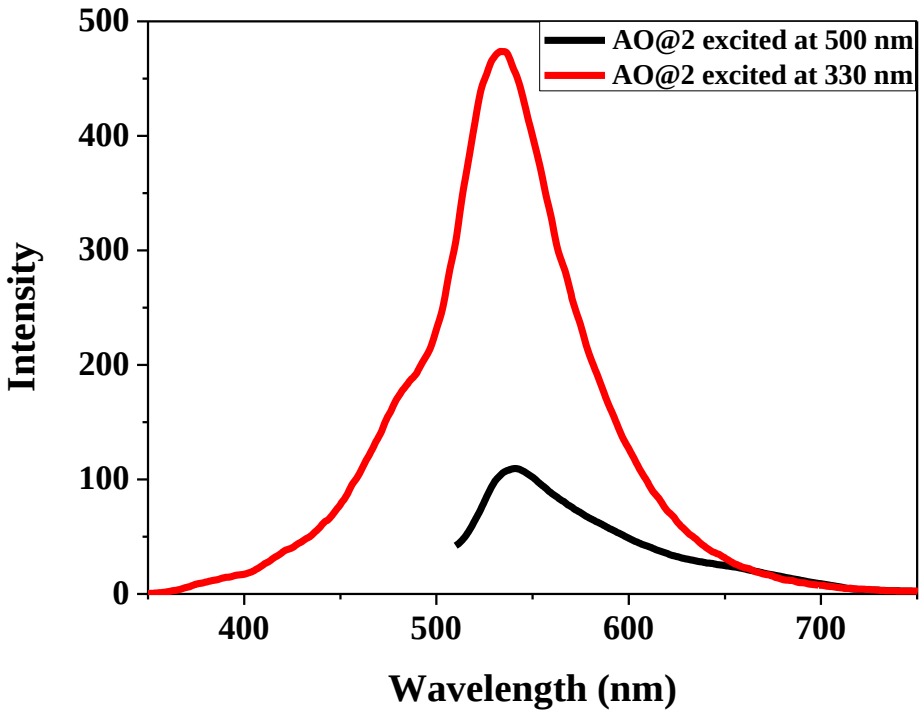

Fig. S19 Emission spectra of **AO@2** upon excitation at 330 and 500 nm.

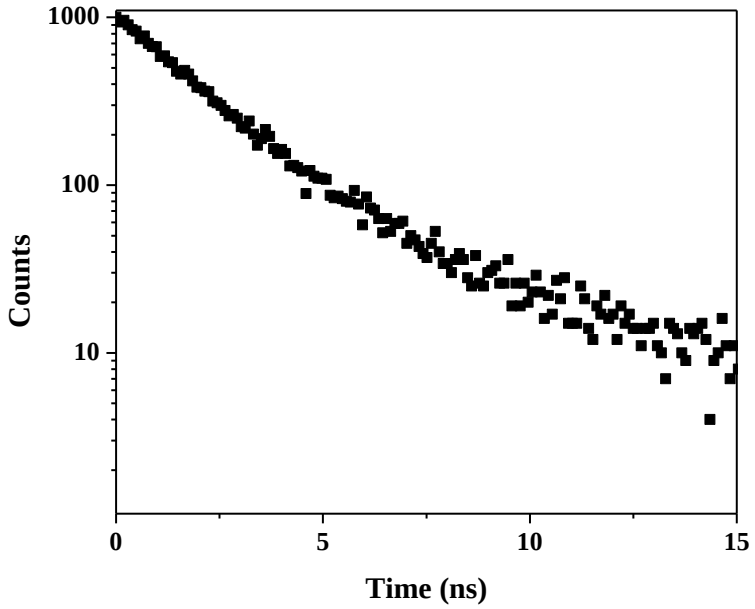

Fig. S20 Fluorescence life time profiles of **AO@2** monitored at 600 nm upon excitation at 405 nm.

Indexing Results of compound 2a

NUMBER OF SINGLE INDEXED LINES = 15

TOTAL NUMBER OF LINES = 17

a = 15.018140 (0.014754) Å α = 90.000000 .000000 °

b = 13.149670 (0.016752) Å β = 98.234620 .083901 °

c = 9.790491 (0.028959) Å γ = 90.000000 .000000 °

UNIT CELL VOLUME = 1913.53 Å^3

H	K	L	SST-OBS	SST-CALC	DELTA	2TH-OBS	2TH-CALC	D-OBS	FREE PARAM.
1	0	0	.002670	.002686	-.000016	5.924	5.941	14.9073	0

-1	0	1	.007825	.007826	-.000001	10.150	10.150	8.7083	0
1	0	1	.010194	.010186	.000008	11.590	11.585	7.6292	0
-1	1	1	.011244	.011257	-.000013	12.174	12.181	7.2643	0
1	1	1	.013579	.013618	-.000039	13.383	13.403	6.6105	0
			0	2	0	.013726		13.456	
1	2	0	.016399	.016412	-.000013	14.715	14.721	6.0152	0
-2	1	1	.018160	.018135	.000025	15.489	15.479	5.7161	0
2	0	1	.019285	.019424	-.000139	15.965	16.023	5.5469	0
2	1	1	.023000	.022855	.000145	17.446	17.391	5.0792	0
-3	0	1	.026957	.026952	.000004	18.900	18.898	4.6917	0
2	2	1	.033143	.033150	-.000007	20.979	20.981	4.2312	0
-4	0	1	.044570	.044574	-.000004	24.375	24.377	3.6487	0
			4	1	1	.057447		27.735	
1	4	0	.057707	.057591	.000117	27.799	27.771	3.2066	0
			-3	3	1	.057836		27.831	
			.064463			29.416	3.0339	0	
-3	4	2	.097272	.097276	-.000005	36.346	36.347	2.4698	0

NUMBER OF OBS. LINES = 17

NUMBER OF CALC. LINES = 17

M(15)= 8 AV.EPS.= .0000383

F 15 = 7.(.015260, 152)

2 LINES ARE UNINDEXED

M-TEST= 8 UNINDEXED IN THE TEST= 1