Supplementary Information

Coordination polymers based on di-9,10-(pyridine-4-yl)-anthracene: selectively adsorbing CO_2 and fluorescent properties

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Table 1. Crystal and Structure Refinement Data for compound **1-4.**

	1	**2**	**3**	**4**
Empirical formula	$C_{26}H_{16}CoNO_4$	$C_{80}H_{44}Co_2N_2O_8$	$C_{24}H_{16}Cd_{0.5}Cl_2N_2$	$C_{24}H_{20}CdCl_2N_2O_2$
Formula weight	465.33	1220.15	459.51	551.72
Temperature (K)	296	296	295	297
Diffrn. wavelength (Å)	0.71073	0.71073	0.71076	0.71073
Crystal system	tetragonal	triclinic	triclinic	monoclinic
Space group	*I*4/*m*	*P*-1	*P*-1	$P2_1/c$
a (Å)	15.208(1)	17.807(3)	8.942(7)	13.403(3)
b (Å)	15.208(2)	19.530(3)	10.101(8)	8.610(2)
c (Å)	18.172(2)	19.611(4)	12.964(10)	9.713(2)
a (°)	90	95.97(5)	88.57(2)	90
β (°)	90	114.76(4)	89.81(3)	97.52(6)
γ (°)	90	90.71(4)	83.80(4)	90
V, Å^3	4202.6(10)	6147.8(18)	1163.7(16)	1111.3(4)
Z	4	2	2	2
ρ_{calc} Mg/m^3	0.735	0.693	0.494	1.649
μ, mm^{-1}	0.425	0.302	0.96	1.247
F(000)	952	1320	157	552
Refl. collected	16225	49862	5654	8814
Independent refl.	2141	27742	3801	2607
Final R indices(R_1)	0.0456	0.0419	0.01065	0.0318
(all data) wR_2	0.1612	0.0905	0.3545	0.0761
GOOF	1.010	1.006	1.553	1.038

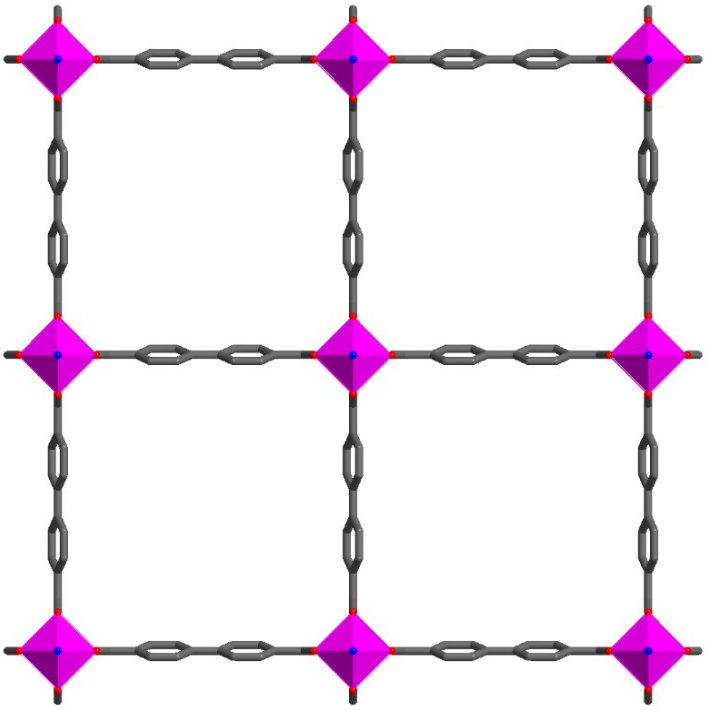

Figure S1. A diagram showing the $Co_2(bpda)_2$ (*bpda* = 4,4′-biphenyldicarboxyic acid) layer structure in **1** (C, grey; O, red; Co, pink).

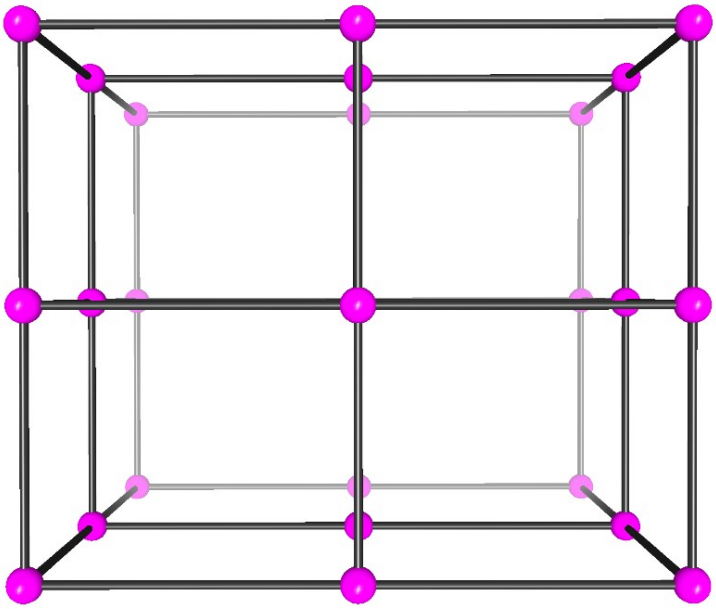

Figure S2. A diagram showing the topology of ***pcu*** for the 3D network in **1** following the classification from *RCSR* (reticular chemistry structure resource, the binuclear Co_2 units are shown as pink balls and organic ligands are shown as dark gray sticks).

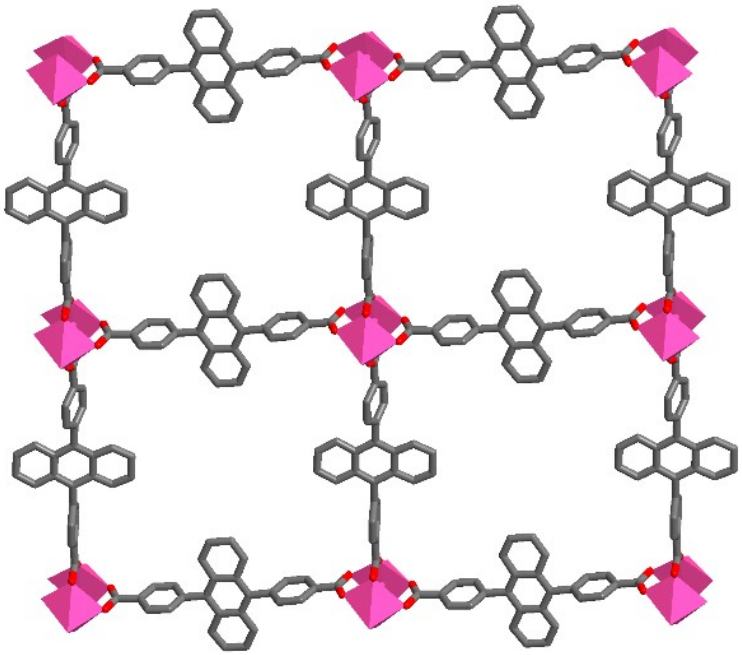

Figure S3. The $Co_2(dcpa)_2$ (*dcpa* = 9,10-Di(4-carboxyphenyl)anthracene) layer structure in **2** (C, grey; O, red; Co, pink polyhedron).

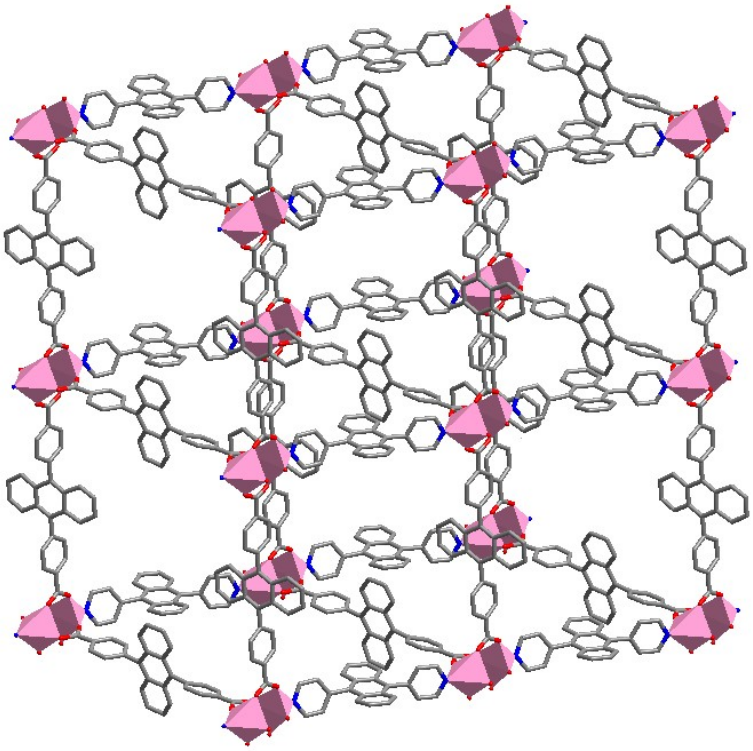

Figure S4. The 3-dimensional open network in **2** (C, grey; O, red; N, blue; Co, pink polyhedron).

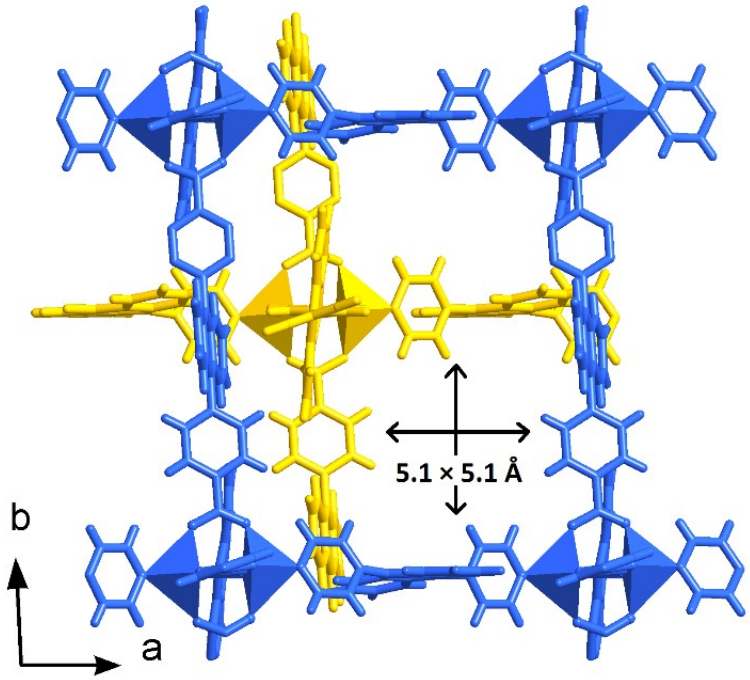

Figure S5. 1D channel of pore size of 5.1 × 5.1 Å along the *c* direction formed between two interpenetrated networks in **2**.

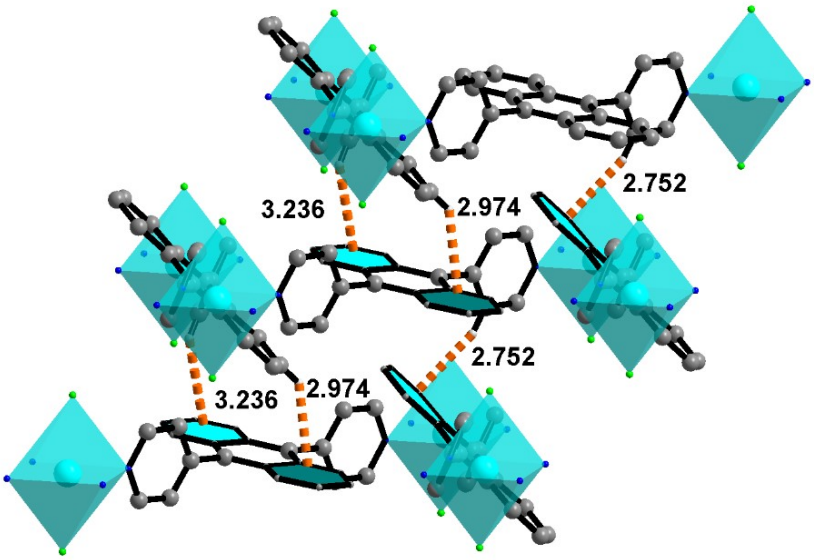

Figure S6. The C-H···π interactions formed between the pyridyl and anthracene groups, and between anthracene groups from adjacent layers in **3** (C, gray; H, light gray; N, blue; Cd, cyan; Cl, green, C-H···π interactions are shown in orange dashed lines).

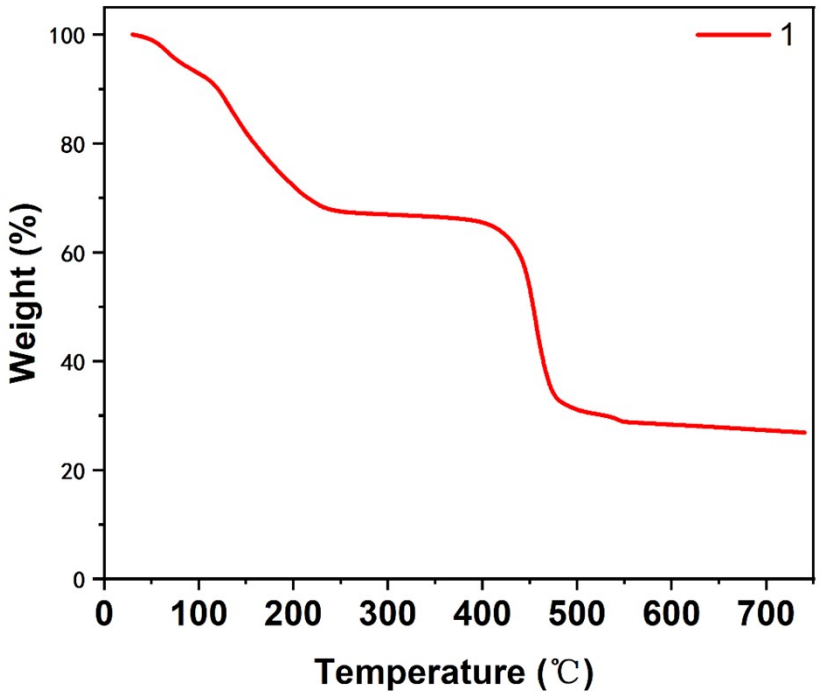

Figure S7. TG profile of **1**.

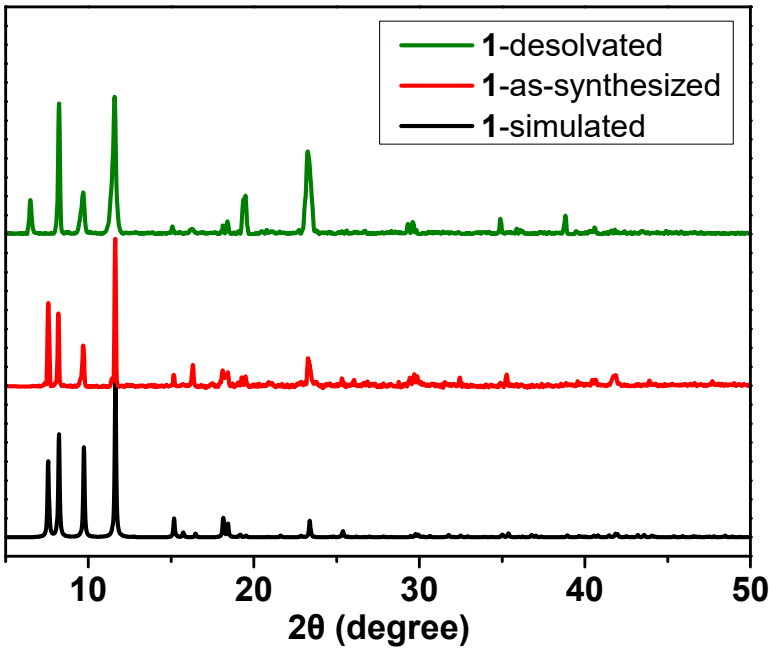

Figure S8. Powder XRD of as-synthesized and de-solvated sample of **1**.

Estimation of pore volume of 1 based on single-crystal structure of as-synthesized sample

The accessible volume calculated by *PLATON* is 2057 $Å^3$ (2.057 *10^{-21} cm^3) per unit cell using a probe of radius of 1.2 Å.

The mass of one unit cell is 3.088 * 10^{-21} g without solvent guests (crystal_density_diffrn is 0.735 $g \cdot cm^{-3}$, unit cell volume is 4202 $Å^3$ (4.202 * 10^{-21} cm^3), 0.735 * 4.202 * 10^{-21} = 3.088 * 10^{-21} g).

The pore volume of **1** calculated based on single crystal structure of as-synthesized sample is 0.666 $cm^3 \cdot g^{-1}$ (2.057 *10^{-21} cm^3 / 3.088 * 10^{-21} g).

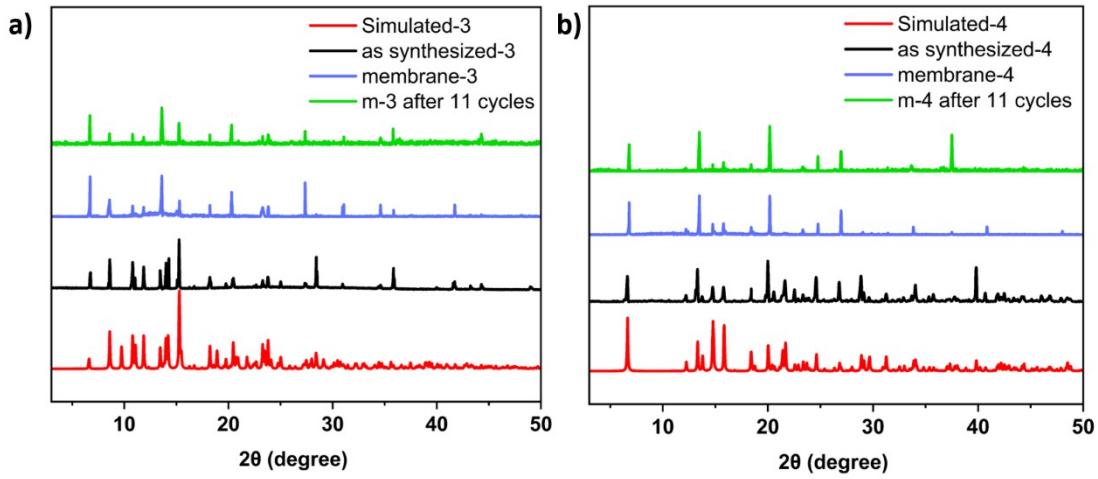

Figure S9. (a) (b) Powder XRD of sample **3**, **4** and **m-3, m-4** and **m-3, m-4** after 11 cycles of detecting tests.

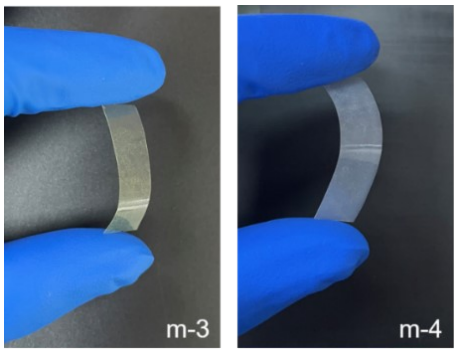

Fig. S10 The picture of **m-3** and **m-4**.

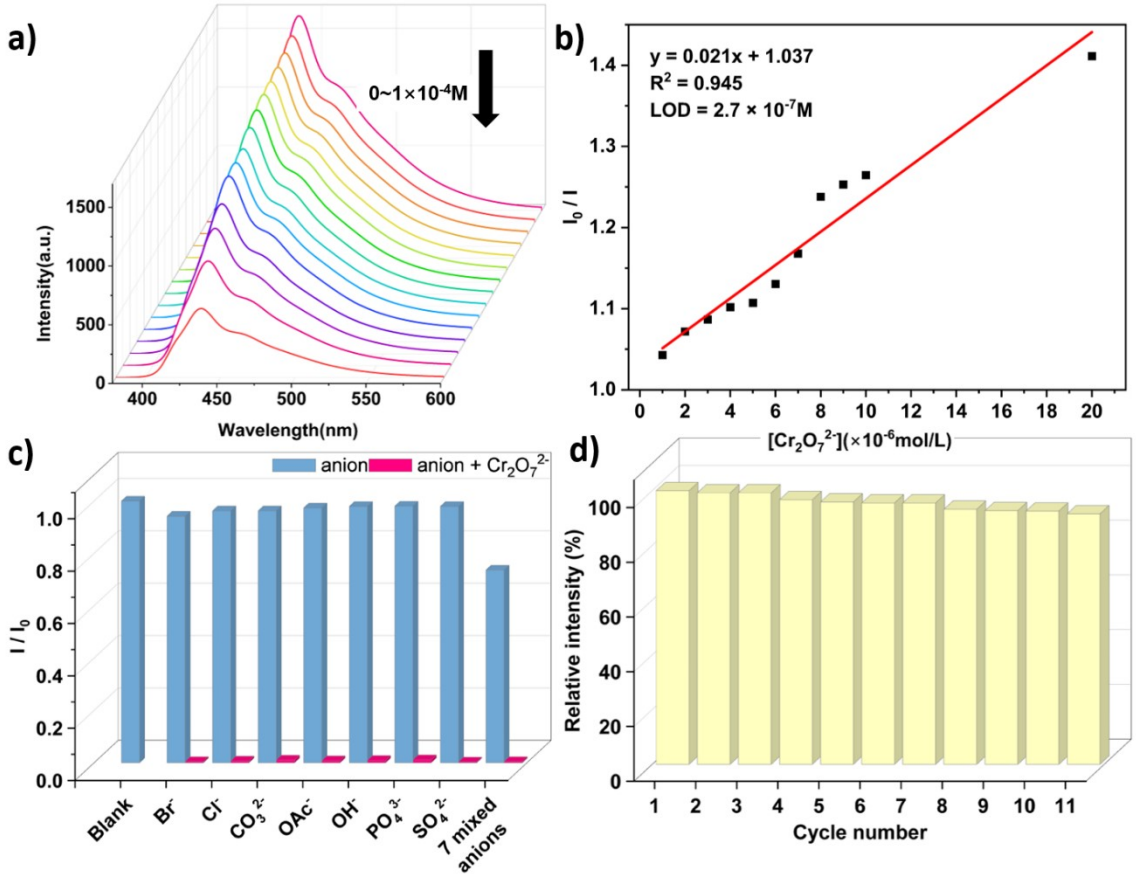

Fig. S11 (a) Fluorescence quenching of **m-4** towards different concentrations of the $Cr_2O_7^{2-}$ solution (**0~1.0×10^{-4}** mol · L^{-1}, λ_{ex} = 365 nm). (b) Stern–Volmer plot of I_0/I vs. concentration of the $Cr_2O_7^{2-}$solution for **m-4**. (c) Relative fluorescence intensity of **m-4** dispersed in aqueous solutions of interfering anions (blue) and subsequent addition of $Cr_2O_7^{2-}$ (pink). (d) The variations of relative fluorescence intensity of **m-4** for detecting $Cr_2O_7^{2-}$ under 11 cycles.

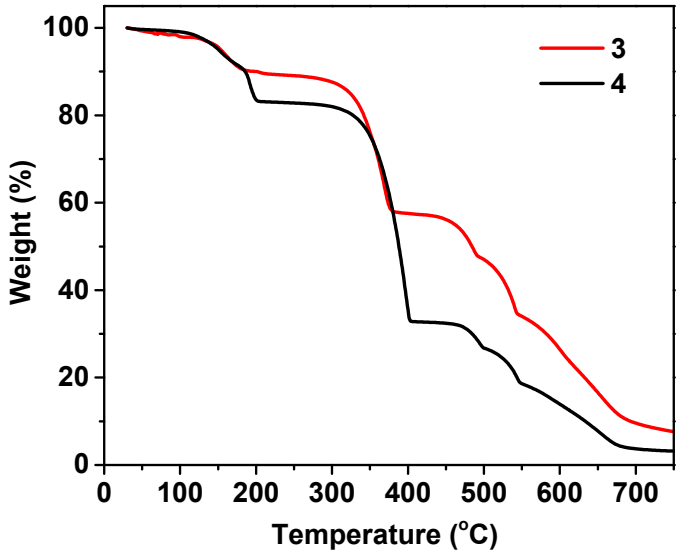

Fig. S12. TG curves for complexes **3** and **4**.

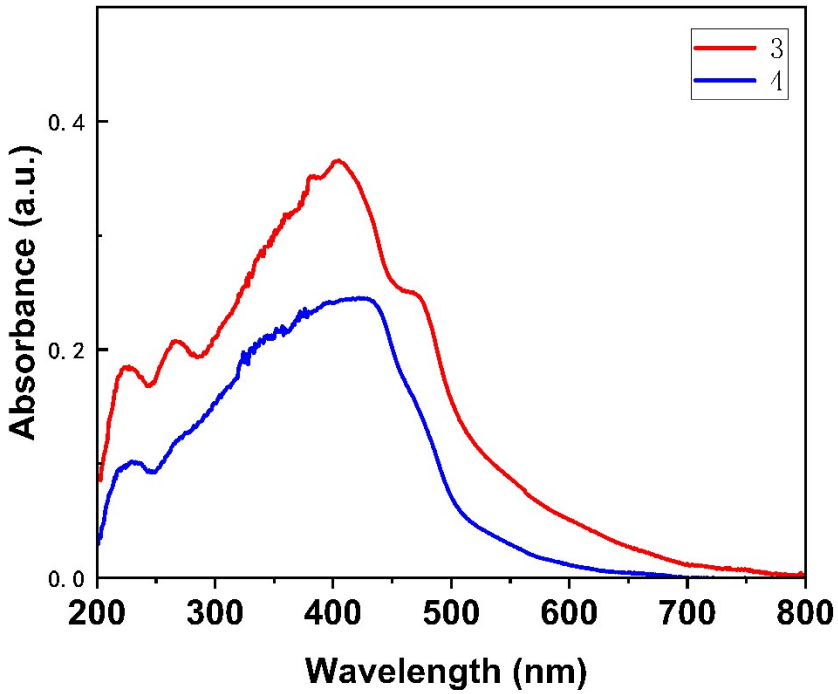

Fig. S13. The Solid UV absorption spectra of 3 and 4.

Preparation of mixed matrix membranes m-3 and m-4:

Submicron CPs particles were prepared according to the reference with slight modifications, [1,2,3] and the preparation procedures of **m-3** and **m-4** were the same. The crystals of 3 (50 mg) are soaked in liquid nitrogen for 20 min and then ground with an agate mortar. The ground sample is then dispersed in dichloromethane (DCM, 10 ml), where a small fraction of the micron-sized crystals was settled while most of the submicron-sized crystals remain in suspension and are subsequently sucked out and vacuum-dried at room temperature. Then, dissolve PMMA (0.3g) in acetone (3.0mL) and sonicated for 30 minutes to obtain a viscous solution. Submicron crystal 3 (0.03g) was added to the acetone solution of PMMA, followed by ultrasonic for 30 minutes to obtain a homogeneous dispersion uniform solution, and finally the solution was dropwise cast onto a glass plate and scraped flat with a spatula, and dried overnight at room temperature to obtain an unsupported film.

Reference

1 G. P. Liu, V. Chernikova, Y. Liu, K. Zhang, Y. Belmabkhout, O. Shekhah, C. Zhang, S. L. Yi, M. Eddaoudi and W. J. Koros, *Nat. Mater*., 2018, **17**, 283.

2 R. J. Lin, L. Ge, L. Hou, E. Strounina, V. Rudolph and Z. H. Zhu, *ACS Appl. Mater. Interfaces*, 2014, **6**, 5609.

3 X. Zhang, Q. Zhang, D. Yue, J. Zhang, J. T. Wang, B. Li, Y. Yang, Y. J. Cui and G. D. Qian, *Small*, 2018, **14**, 1801563.