Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

A 2D porous pentiptycene-based MOF for efficient detection of Ba^{2+} and selective adsorption of dyes from water

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1. ^{1}H NMR spectrum of ligand H_2L.

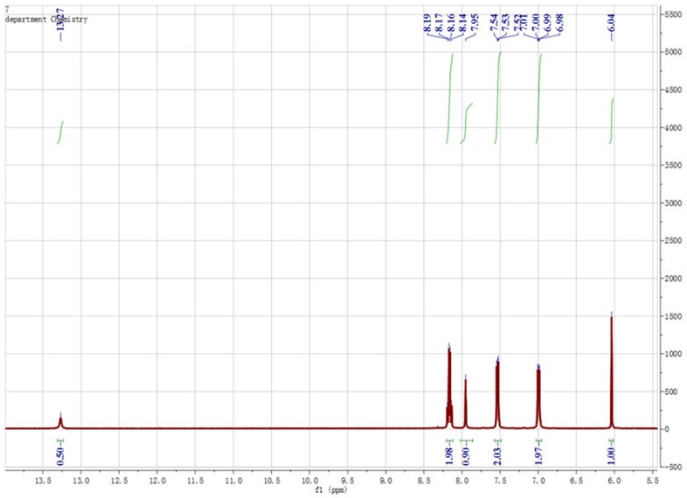

Figure S1. ^{1}H NMR spectrum of ligand H_2L.

2. Crystal structure.

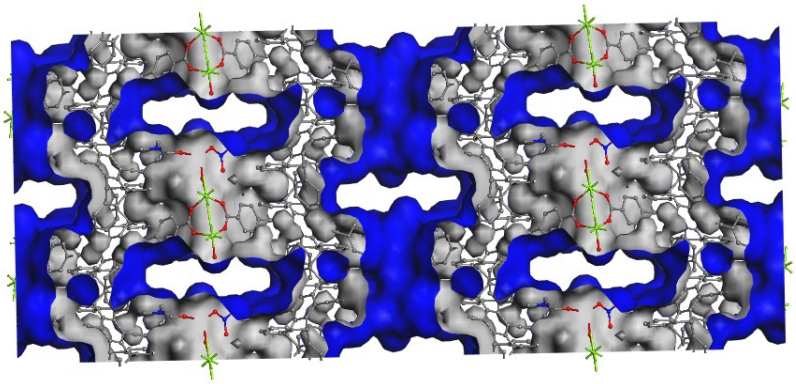

Figure S2. Connolly surface representation along the *a* axis.

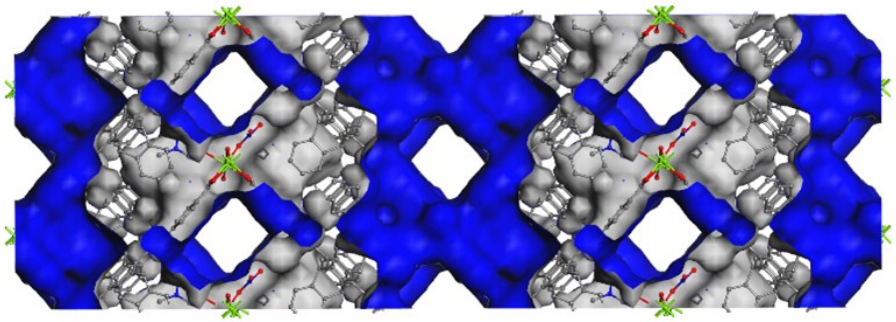

Figure S3. Connolly surface representation along the *c* axis.

3. Powder X-ray diffraction and thermogravimetric analysis.

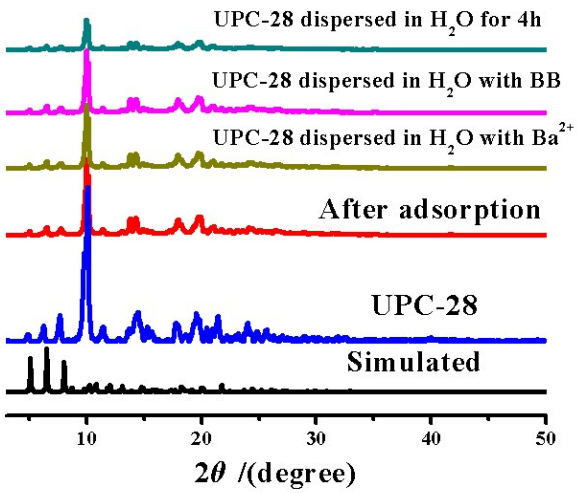

Figure S4. PXRD patterns of **UPC-28**.

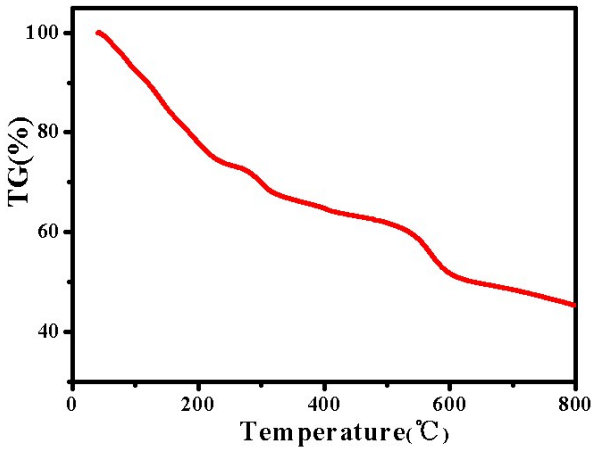

Figure S5. The TGA curve for **UPC-28**.

4. Crystal data for UPC-28.

Table S1: Crystal Data for **UPC-28**

Identification code	**UPC-28**
Empirical formula	$C_{114}H_{80}Mg_3N_2O_{18}$
Formula weight	1838.73
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.8132(2)
b/Å	34.5225(5)
c/Å	14.9681(3)
α/°	90.00
β/°	101.5443(18)
γ/°	90.00
Volume/Å^3	5980.80(19)
Z	2
*ρ*calcg/cm^3	1.021
μ/mm^{-1}	0.701
F(000)	1916.0
Reflections collected	21771
Independent reflections	10657 [R_{int} = 0.0230, R_{sigma} = 0.0343]
Data/restraints/parameters	10657/0/623
Goodness-of-fit on F2	1.081
Final R indexes [I>=2σ (I)]	R_1 = 0.0759, wR_2 = 0.2256
Final R indexes [all data]	R_1 = 0.0866, wR_2 = 0.2379
Largest diff. peak/hole / e Å-3	1.79/-0.81

$R_1 = \Sigma| |F_o|-|F_c| |/ \Sigma|F_o|$, $wR_2 = [\Sigma w(F_o^2-F_c^2)^2]/ \Sigma w(F_o^2)^2]^{1/2}$

5. Selected bond lengths (Å) and angles (º) for UPC-28.

Table S2: Selected bond lengths (Å) and angles (º) for **UPC-28**

Mg1—Mg2^{i}	3.6488 (11)	Mg1—Mg2	3.6488 (11)
Mg1—O1	2.0510 (17)	Mg1—O1^{i}	2.0510 (17)
Mg1—O2	2.0768 (19)	Mg1—O2^{i}	2.0768 (18)
Mg1—O4	2.145 (2)	Mg1—O4^{i}	2.145 (2)
Mg2—O3^{ii}	2.039 (2)	Mg2—O4	2.150 (2)
Mg2—O5	2.016 (2)	Mg2—O6	2.093 (2)
Mg2—O7	2.074 (2)	Mg2—O16	2.074 (3)
Mg2^{i}—Mg1—Mg2	180.0	O1^{i}—Mg1—Mg2^{i}	70.99 (7)
O1^{i}—Mg1—Mg2	109.01 (7)	O1—Mg1—Mg2^{i}	109.02 (7)
O1—Mg1—Mg2	70.98 (7)	O1—Mg1—O1^{i}	180.0
O1—Mg1—O2^{i}	92.33 (8)	O1^{i}—Mg1—O2	92.33 (8)
O1—Mg1—O2	87.67 (8)	O1^{i}—Mg1—O2^{i}	87.67 (8)
O1—Mg1—O4^{i}	87.20 (8)	O1^{i}—Mg1—O4	87.20 (8)
O1^{i}—Mg1—O4^{i}	92.80 (8)	O1—Mg1—O4	92.80 (8)
O2^{i}—Mg1—Mg2	110.88 (7)	O2—Mg1—Mg2^{i}	110.88 (7)
O2—Mg1—Mg2	69.12 (7)	O2^{i}—Mg1—Mg2^{i}	69.12 (7)
O2—Mg1—O2^{i}	180.00 (9)	O2—Mg1—O4^{i}	87.54 (9)
O2^{i}—Mg1—O4	87.54 (9)	O2^{i}—Mg1—O4^{i}	92.46 (9)
O2—Mg1—O4	92.46 (9)	O4^{i}—Mg1—Mg2	148.11 (6)
O4—Mg1—Mg2^{i}	148.11 (6)	O4^{i}—Mg1—Mg2^{i}	31.89 (6)
O4—Mg1—Mg2	31.89 (6)	O4—Mg1—O4^{i}	180.0
O3^{ii}—Mg2—Mg1	68.83 (7)	O3^{ii}—Mg2—O4	92.02 (9)
O3^{ii}—Mg2—O6	88.99 (9)	O3^{ii}—Mg2—O7	175.58 (12)
O3^{ii}—Mg2—O16	87.44 (11)	O4—Mg2—Mg1	31.80 (6)
O5—Mg2—Mg1	70.52 (8)	O5—Mg2—O3^{ii}	91.34 (10)
O5—Mg2—O4	90.67 (10)	O5—Mg2—O6	178.15 (12)
O5—Mg2—O7	92.68 (10)	O5—Mg2—O16	89.71 (12)
O6—Mg2—Mg1	111.29 (8)	O6—Mg2—O4	91.14 (9)
O7—Mg2—Mg1	114.32 (10)	O7—Mg2—O4	89.77 (11)
O7—Mg2—O6	86.93 (10)	O7—Mg2—O16	90.74 (13)
O16—Mg2—Mg1	148.04 (9)	O16—Mg2—O4	179.34 (10)
O16—Mg2—O6	88.48 (12)	Mg1—O4—Mg2	116.31 (9)

6. Gas sorption for UPC-28.

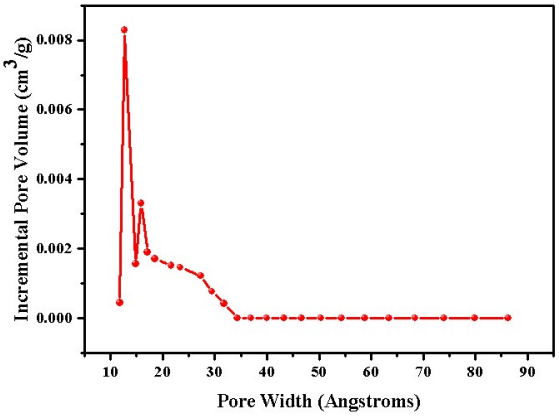

Figure S6. The pore size distribution of **UPC-28**.

Table S3: Equation parameters for the single-site Langmuir-Freundlich model.(CO_2/N_2)

Adsorbates	a (mmol/g)	b (kPa^{-1})	c	R^2
CO_2	8.42992	0.00324	0.95741	1
N_2	0.25856	0.00431	1.13565	0.99952

Table S4: Equation parameters for the single-site Langmuir-Freundlich model.(CO_2/CH_4)

Adsorbates	a (mmol/g)	b (kPa^{-1})	c	R^2
CO_2	8.42992	0.00324	0.95741	1
CH_4	3.92289	0.00162	1.00498	0.99999

Table S5: Equation parameters for the single-site Langmuir-Freundlich model.(C_2H_2/CH_4)

Adsorbates	a (mmol/g)	b (kPa^{-1})	c	R^2
C_2H_2	174.31333	0.000231	0.75931	0.99706
CH_4	3.92289	0.00162	1.00498	0.99999

Table S6: Equation parameters for the single-site Langmuir-Freundlich model.(C_2H_2/ C_2H_6)

Adsorbates	a (mmol/g)	b (kPa^{-1})	c	R^2
C_2H_2	174.31333	0.000231	0.75931	0.99706
C_2H_6	0.71729	0.003	1.2934	0.9966

Table S7: Equation parameters for the single-site Langmuir-Freundlich model.(C_3H_6/ C_3H_8)

Adsorbates	a (mmol/g)	b (kPa^{-1})	c	R^2
C_3H_6	1.27756	0.00232	1.34523	0.99728
C_3H_8	1.87636	0.0001158	1.58799	0.99357

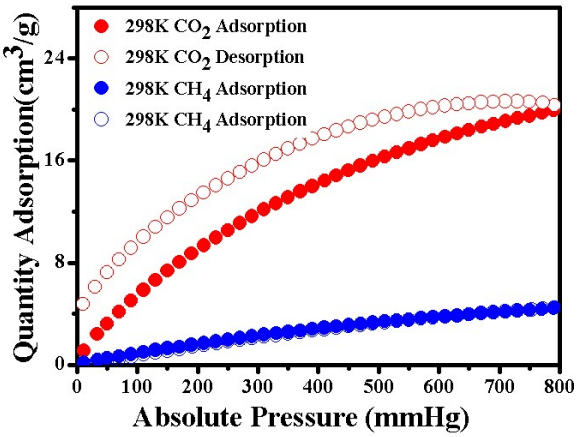

Figure S7. The CO_2 and CH_4 adsorption capacity for **UPC-28** at 298K.

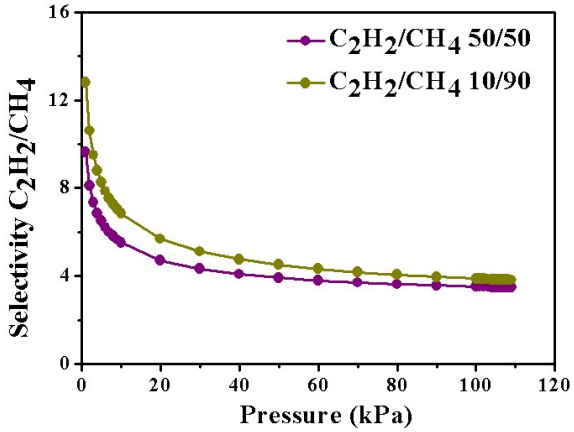

Figure S8. The C_2H_2/ CH_4 selectivity for **UPC-28** at 273 K calculated by the IAST method for two C_2H_2 concentrations (C_2H_2/ CH_4: 10/90 and 50/50) in C_2H_2/ CH_4 binary mixtures.

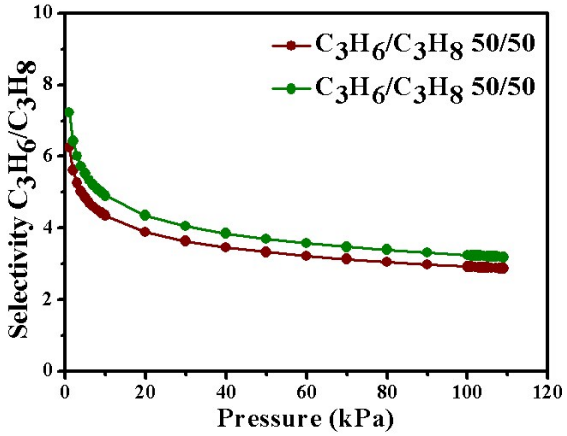

Figure S9. The C_3H_6/ C_3H_8 selectivity for **UPC-28** at 273 K calculated by the IAST method for two C_3H_6 concentrations (C_3H_6/ C_3H_8: 10/90 and 50/50) in C_3H_6/ C_3H_8 binary mixtures.

7. Luminescence spectra of the UPC-28 dispersed in aqueous solutions with different metal ions.

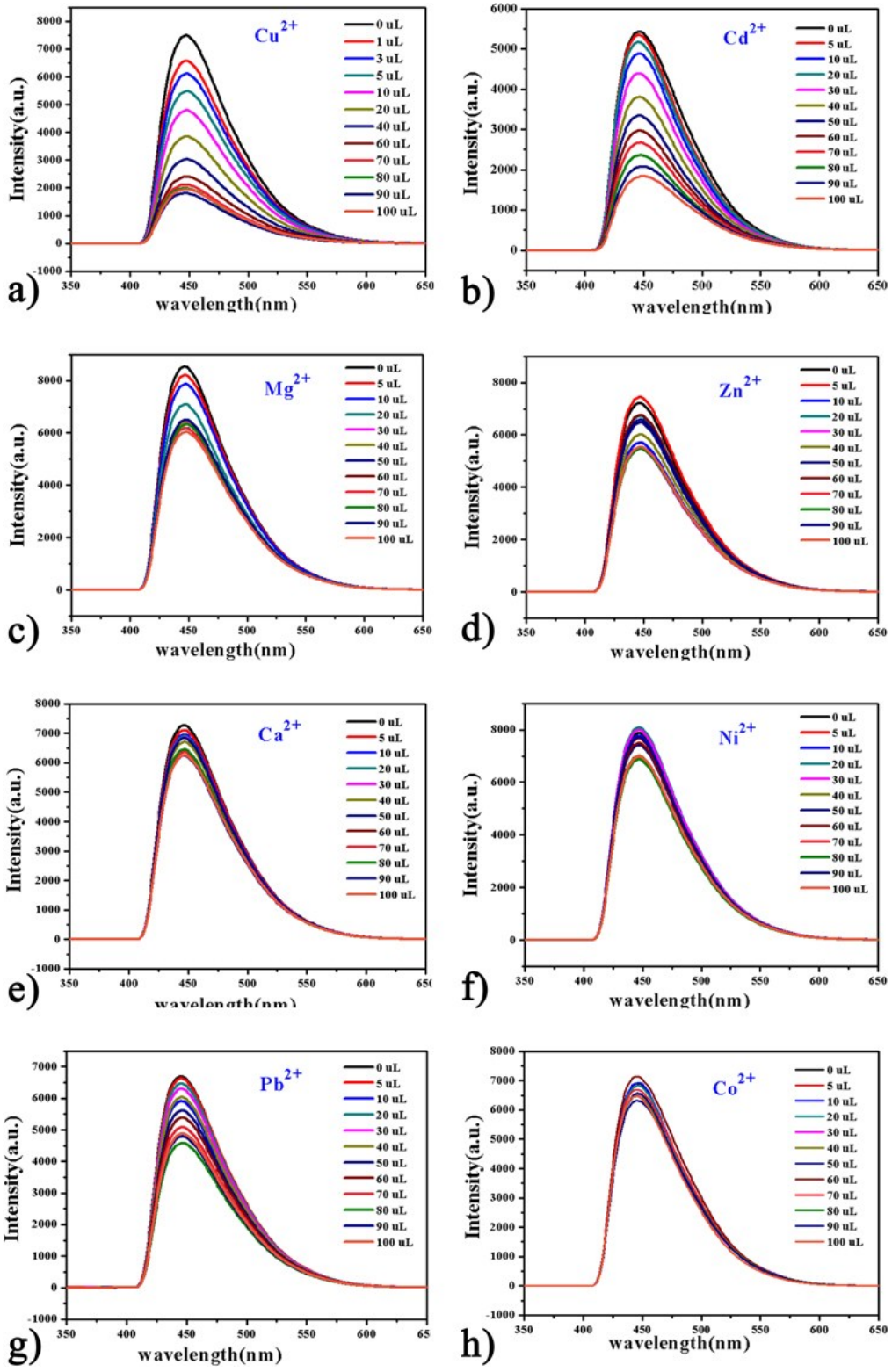

Figure S10. Fluorescent spectra of 2 mg/mL **UPC-28** dispersed in aqueous solution treated with: a) Cu^{2+}, b) Cd^{2+}, c) Mg^{2+}, d) Zn^{2+}, e) Ca^{2+}, f) Ni^{2+}, g) Pb^{2+} and h) Co^{2}

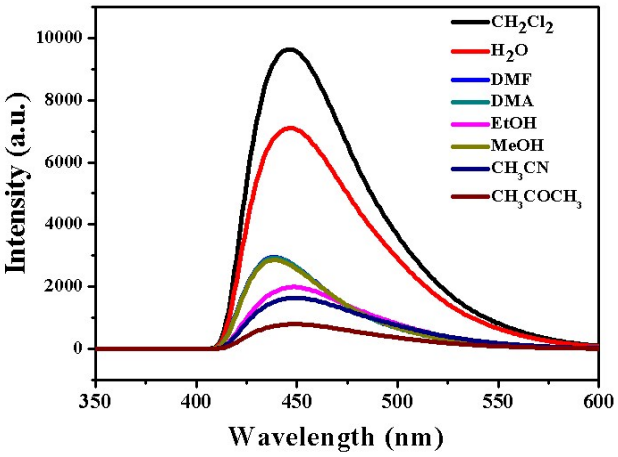

Figure S11. Fluorescent spectra of **UPC-28** dispersed in different solvents.

8. Adsorption of dye molecules.

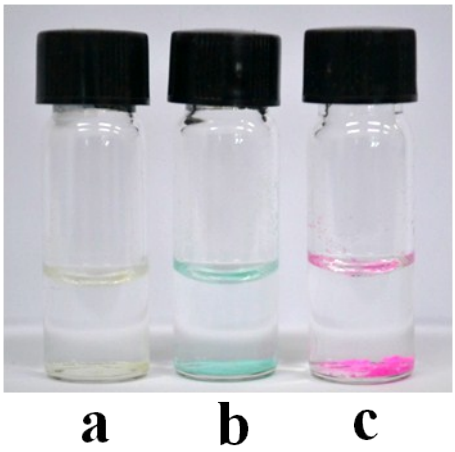

Figure S12. (a) Photographs of **UPC-28** in aqueous solutions; (b) Photographs of **UPC-28** in MB aqueous solutions after interaction; (c) Photographs of **UPC-28** in RhB aqueous solutions after interaction.