

Supporting Information

A new triazine functionalized luminescent covalent organic framework for nitroaromatic sensing and CO₂ storage

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Section S1: Spectroscopic data of the monomers

TAPT:

^1H NMR (DMSO- d_6 , 500 MHz): δ (ppm): 8.35 (d, $J=8.5$, 6H), 6.69 (d, $J=8.5$, 6H), 5.9 (s, 6H).

^{13}C NMR (DMSO- d_6 , 125 MHz): δ (ppm): 169.6, 152.9, 130.1, 122.9, 113.1.

HR-MS m/z : 355.24 (M^+ , calculated for $\text{C}_{21}\text{H}_{18}\text{N}_6$ 354.41)

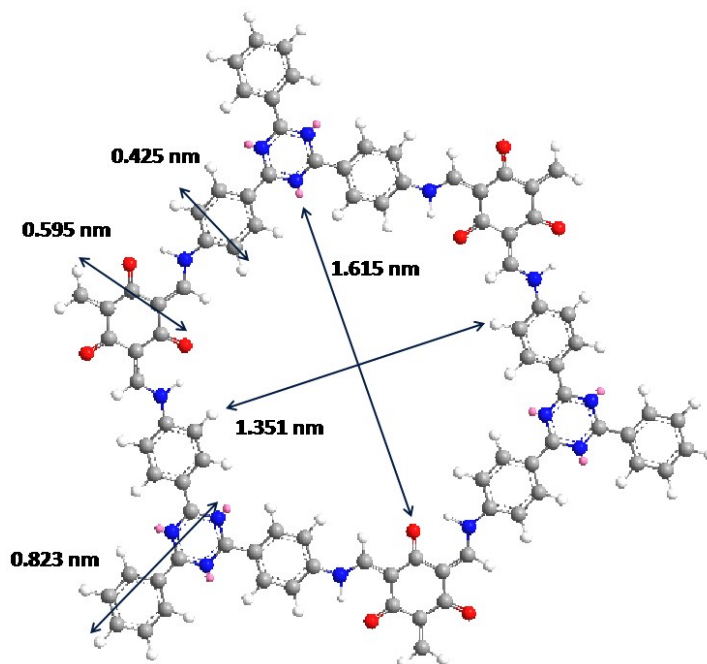
TFP:

^1H NMR (CDCl_3 , 500 MHz): δ (ppm): 14.116 (s, 3H), 10.153 (s, 3H).

^{13}C NMR (CDCl_3 , 125 MHz): 192.20, 173.74, 103.06.

Section S2: Energy minimized structure

The energy minimization job of the hexagonal structure of TRIPTA was performed using chem.3D ultra 12.0 software. The resultant structure is shown below, where the summation of pore size (1.351 nm) and wall thickness (0.425 nm) is 1.776 nm which closely matches with the unit cell parameter 1.755 nm.



Section S3 Physico-chemical properties of TRIPTA

Table S1

Sample	d_{100} (nm)	a_{100} (nm)	S_{BET} (m^2g^{-1})	PD_{NLDFT} (nm)	PV (cm^3g^{-1})
TRIPTA	1.52	1.755	609	1.68	0.351

d_{100} is the d(100) spacing.

a_{100} (unit cell parameter) = $2 d_{100}/\sqrt{3}$.

S_{BET} = BET surface area.

PD_{NLDFT} is average pore diameter using NLDFT method.

PV is the total pore volume.

Section S4: CHN analysis data of TRIPTA

Table S2

TRIPTA	C (%)	H (%)	N (%)	O (%)
Experimental	63.93	4.05	14.97	-
Theoretical	63.77	4.25	14.90	17.00

Section S5: HR-TEM analysis

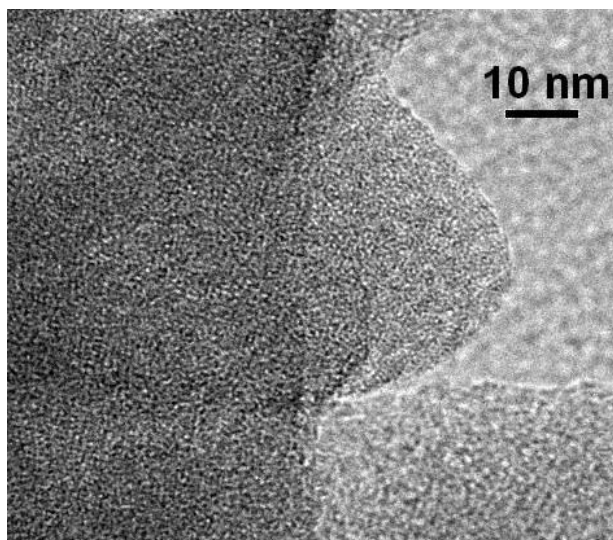


Figure S1. HR-TEM image of covalent organic framework TRIPTA

Section S6: FE-SEM analysis

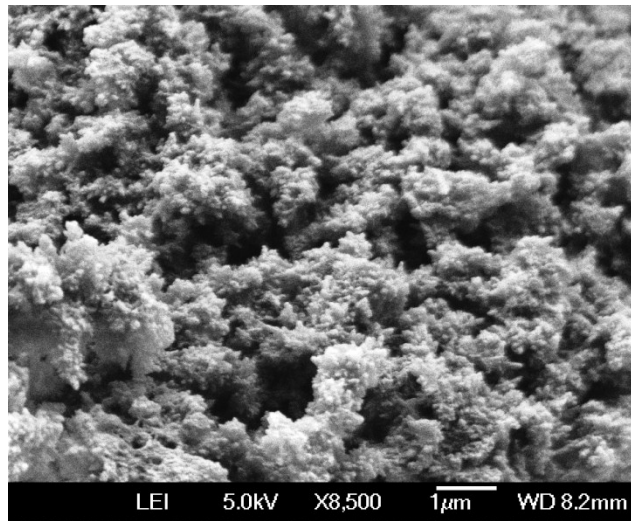


Figure S2. FE-SEM image of TRIPTA

Section S7: Thermogravimetric analysis

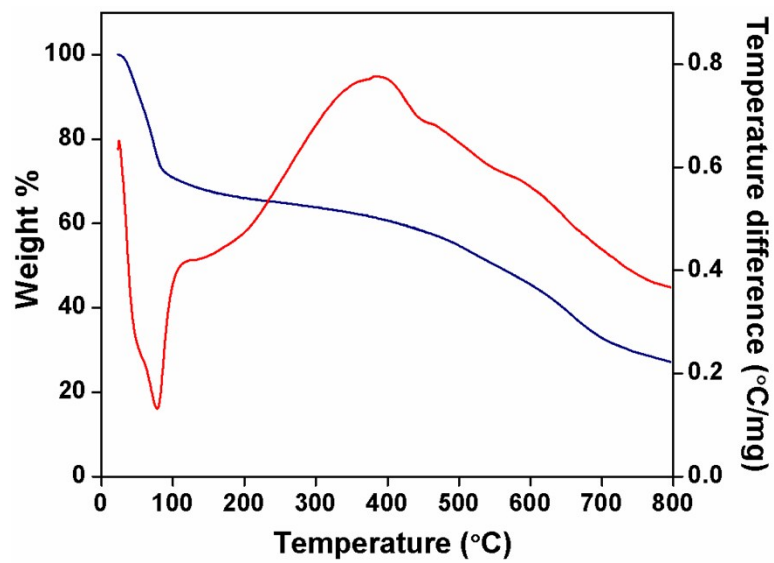


Figure S3. TGA (blue) and DTA (red) plot of TRIPTA

Section S8: Effect of solvent on fluorescence property

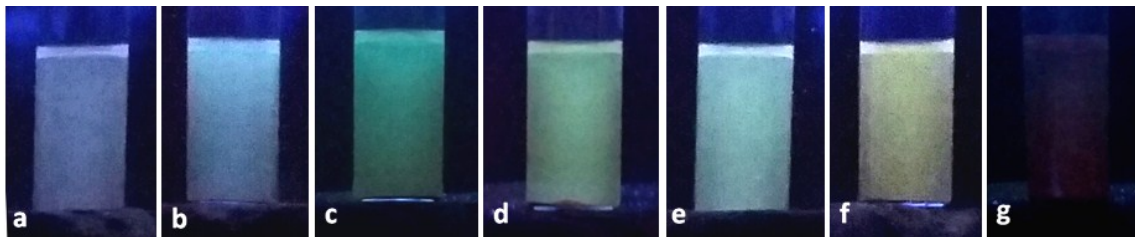


Figure S4. Photographic image of 0.5 mg/mL suspension of TRIPTA in various polar aprotic solvents, (a) chloroform, (b) dichloromethane, (c) tetrahydrofuran, (d) acetone, (e) N,N-dimethylformamide, (f) acetonitrile under UV light ($\lambda_{\text{ex}} = 365 \text{ nm}$). (g) No fluorescence was observed in case of non-polar (cyclohexane, toluene) and polar protic (water, methanol, ethanol) solvents.

Section S9: Fluorescence spectrum of TRIPTA in various solvent

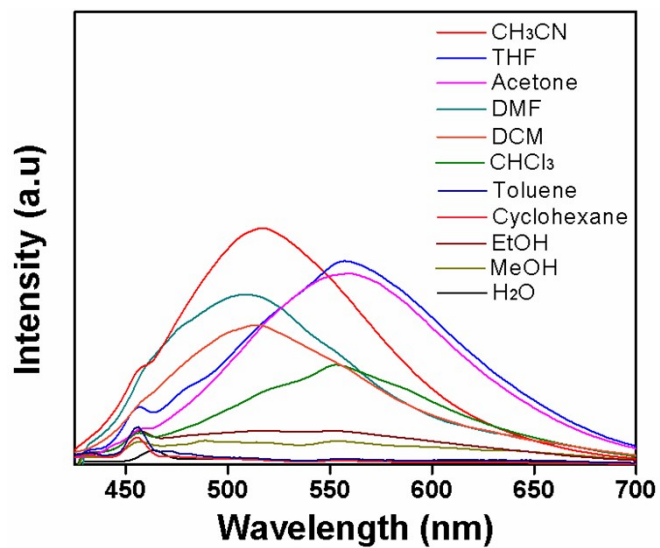


Figure S5. Photoluminescence spectra of TRIPTA suspended in various polar and non-polar solvents ($\lambda_{\text{ex}} = 365 \text{ nm}$).

Section S10: Solid state fluorescence spectrum of TRIPTA

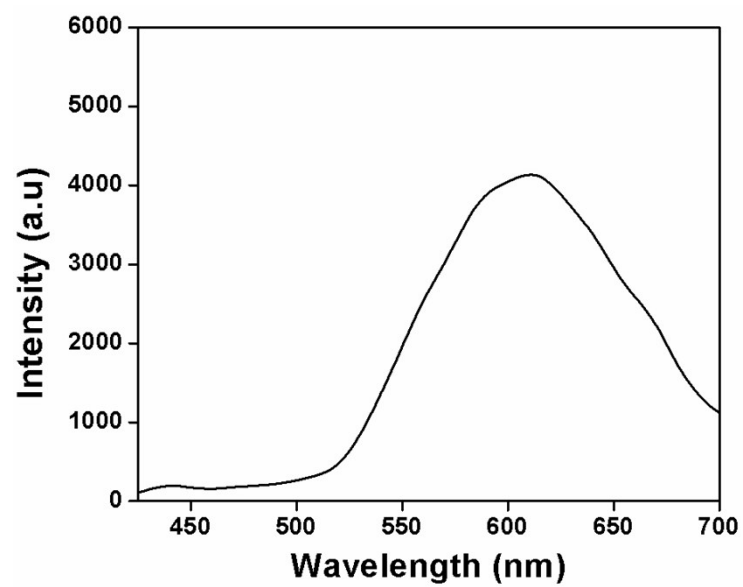


Figure S6. Solid state fluorescence spectrum of TRIPTA ($\lambda_{\text{ex}} = 325$ nm).

Section S11: UV-Vis spectra of acetonitrile suspension of TRIPTA
in presence of TNP

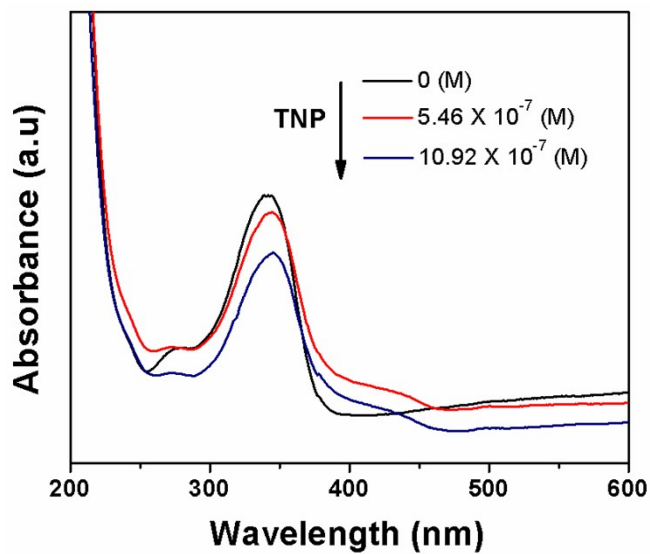


Figure S7. UV-Vis diffuse reflectance spectra of acetonitrile suspension of TRIPTA in presence of TNP

Section S12 TCSPC calculation for average fluorescence lifetime measurement

Table S3

Sample	T1	T2	T3	B1	B2	B3	SumB	A1=[B1 /SumB]	A2=[B2 /SumB]	A3=[B1 /SumB]	<I> (ns)	χ^2
TRIPTA	1.78	5.76	0.09	0.670	0.040	0.257	0.967	0.693	0.041	0.266	1.49	1.094
TRIPTA +TNP	2.21	0.18	7.04	0.108	0.119	0.019	0.246	0.439	0.484	0.077	1.59	1.055
TRIPTA +DNP	0.06	0.76	2.75	0.353	0.055	0.060	0.468	0.754	0.118	0.128	0.49	0.992
TRIPTA +DNT	0.63	2.45	0.05	0.055	0.064	0.483	0.602	0.091	0.106	0.802	0.36	1.052
TRIPTA +NP	0.70	2.45	0.05	0.048	0.056	0.444	0.548	0.088	0.102	0.810	0.35	1.012

Where, $\langle I \rangle = A1T1+A2T2+A3T3$ and χ^2 is the accuracy factor.

Section S13: Recyclability test for the CO₂ capture

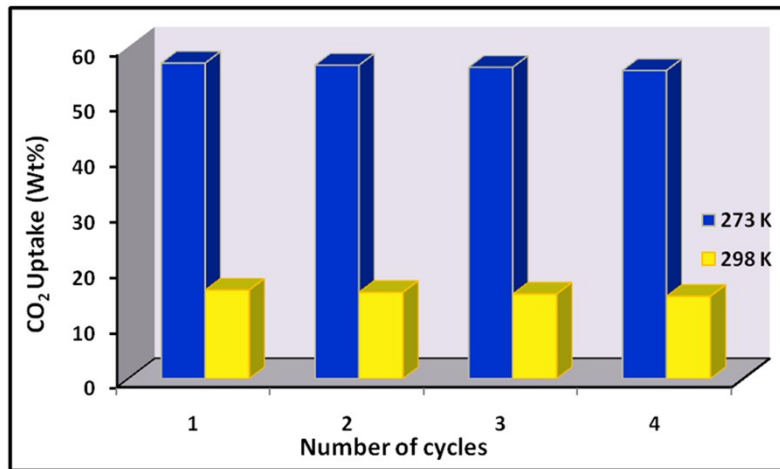


Figure S8. CO₂ adsorption capacity for recycled TRIPTA at 273 K and 298 K, 5 bar pressure