Supporting Information

Multiple stimuli-responsive and reversible fluorescence switches based on a diethylamino-functionalized tetraphenylethene

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1. NMR and MS spectra of TPE-4N

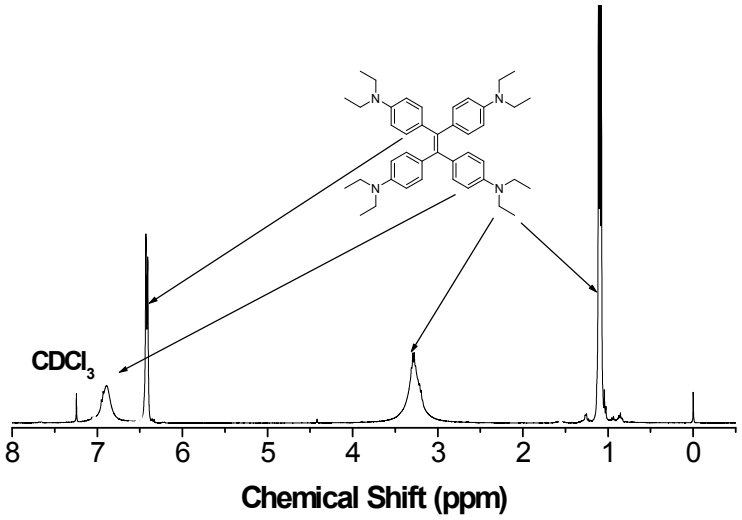

Fig. S1 The NMR spectrum of TPE-4N in $CDCl_3$.

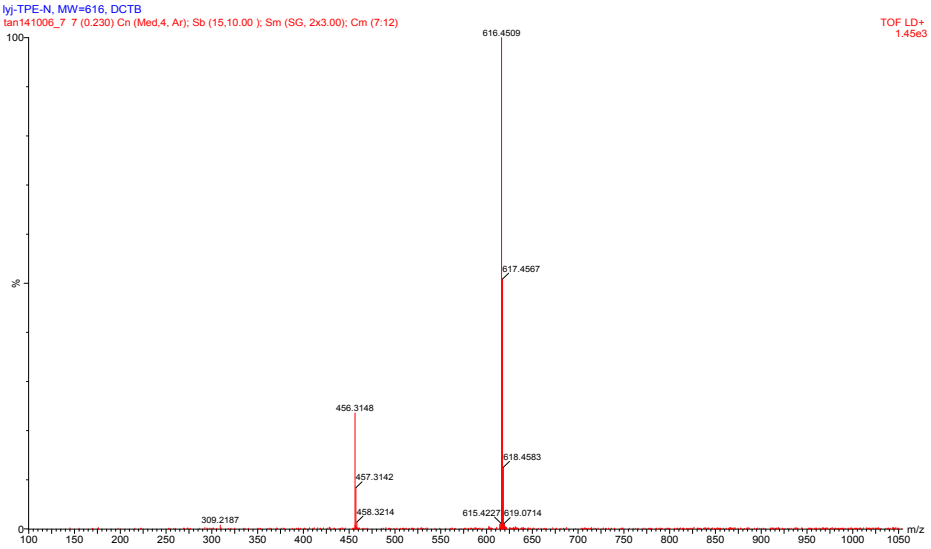

Fig. S2 The MS spectrum of TPE-4N (Mw = 616.45).

2. TPE packing in crystal

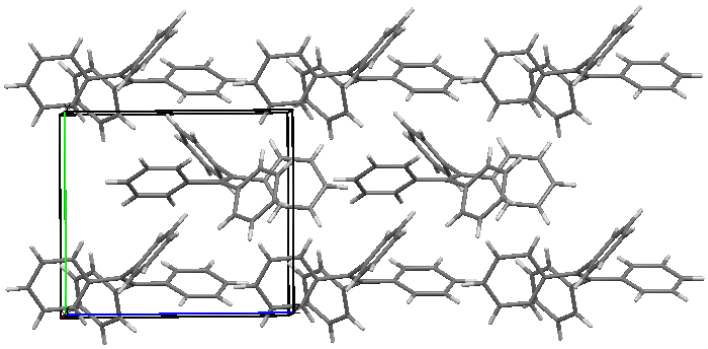

Fig S3 TPE packing in the crystalline state.

3. TPE-4N packing in crystal and its single data

Table S1. Crystal data and structure refinement for TPE-4N(CCDC: 1061949）.

Identification code	TPE-4N	
Empirical formula	C42 H56 N4	
Formula weight	616.91	
Temperature	99.9(4) K	
Wavelength	1.5418 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.9822(9) Å	□= 88.643(4)°.
	b = 17.3332(9) Å	□= 86.828(5)°.
	c = 19.1196(8) Å	□ = 81.890(5)°.
Volume	3597.2(4) $Å^3$	
Z	4	
Density (calculated)	1.139 Mg/m^3	
Absorption coefficient	0.501 mm^{-1}	
F(000)	1344	
Crystal size	0.20 x 0.06 x 0.02 mm^3	
Theta range for data collection	4.07 to 67.49°.	
Index ranges	-13<=h<=13, -18<=k<=20, -22<=l<=13	
Reflections collected	20202	
Independent reflections	12722 [R(int) = 0.0539]	
Completeness to theta = 66.50°	98.66 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.89396	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12722 / 0 / 845	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.0829	
R indices (all data)	R1 = 0.0865, wR2 = 0.0936	
Largest diff. peak and hole	0.233 and -0.204 $e.Å^{-3}$	

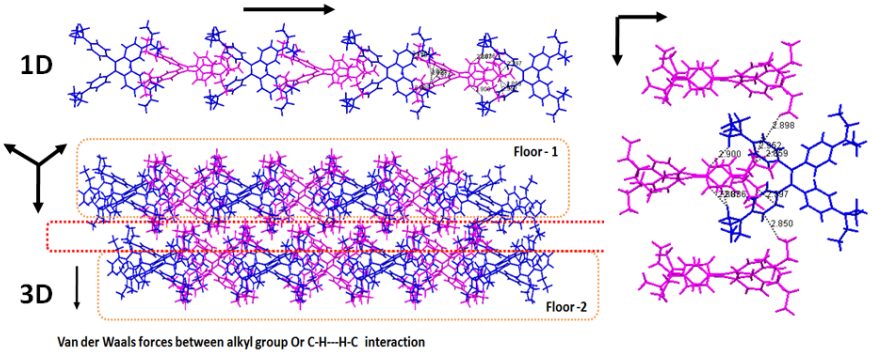

Fig. S4 TPE-4N packing (in 1D, 2D and 3D) in the crystalline state.

4. Solvatochromic absorption and fluorescence spectra

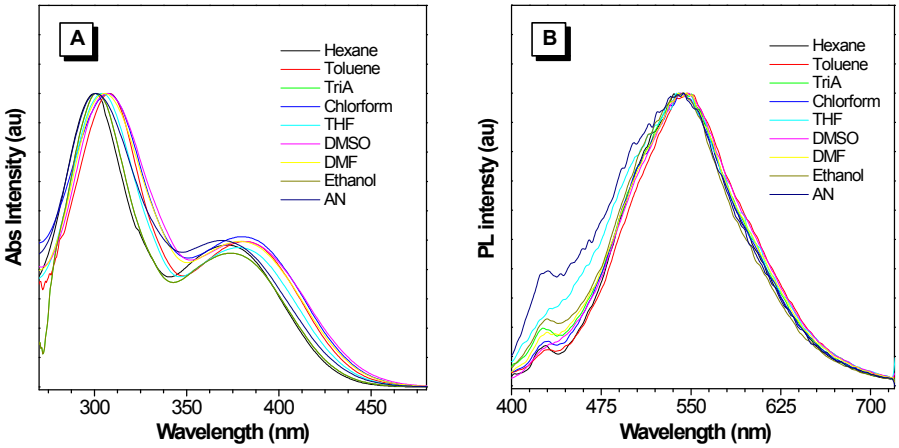

Fig. S5 Solvatochromic absorption and fluorescence in solvents with increased solvent polarities

5. Absorption spectra of TPE-4N in buffers with different pH values

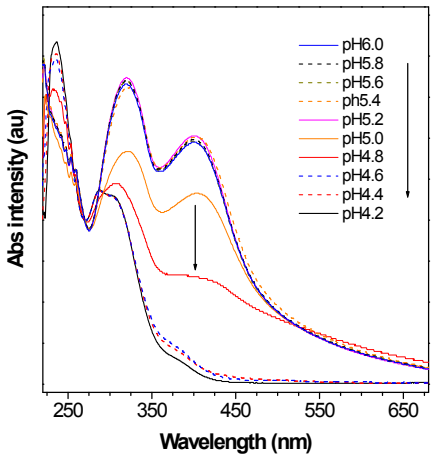

Fig. S6 The absorption spectra of TPE-4N in different buffers with pH values in the range of 4.2–6.0.

6. NMR spectrum of *p*-TPE-4N

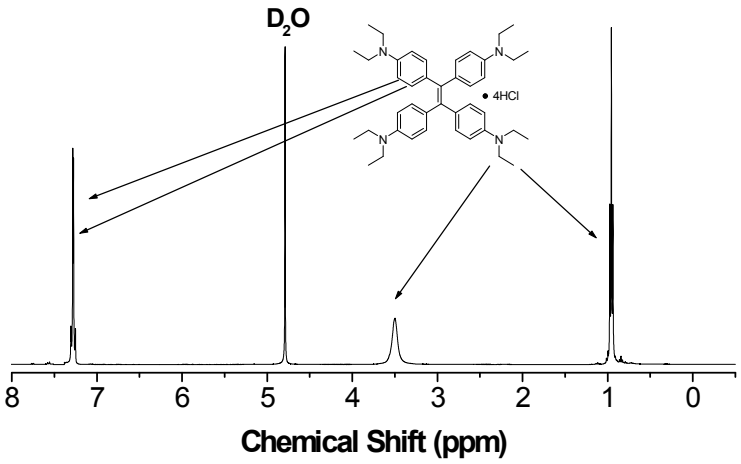

Fig. S7. The NMR spectrum of *p*-TPE-4N in D_2O.