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Redox regulation of electrofluorochromic behavior for AIEgen-doped PVA hydrogel based on ferrocene derivate

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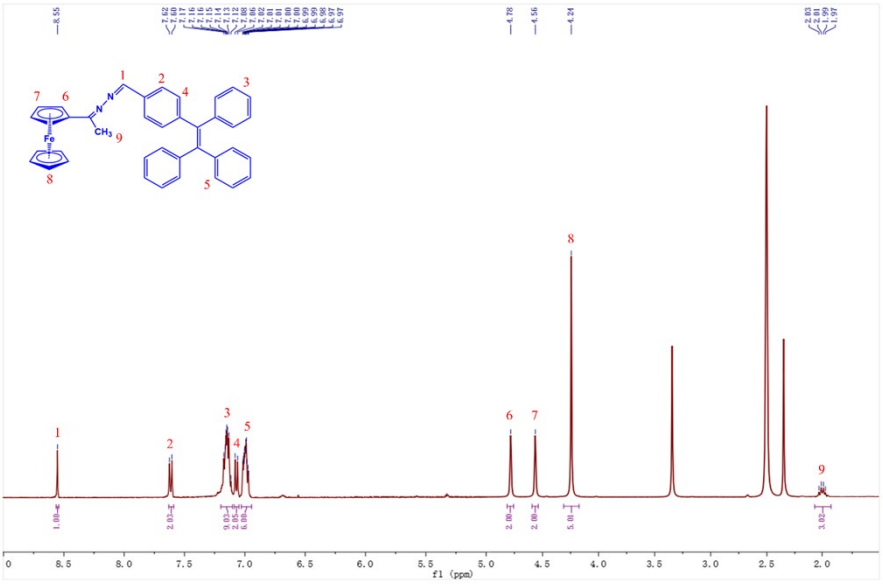


Figure S1 The ^{1}H NMR of FcMe-TPE (DMSO-d_6).

^{1}H NMR (400 MHz, DMSO-d_6): δ 8.55 (s, 1H), 7.61 (d, J = 8.2 Hz, 2H), 7.15 (dt, J = 7.2, 4.7 Hz, 9H), 7.07 (d, J = 8.2 Hz, 2H), 6.99 (tdd, J = 7.4, 5.0, 1.8 Hz, 6H), 4.78 (s, 2H), 4.56 (s, 2H), 4.24 (s, 5H), 2.00 (q, J = 7.0, 6.5 Hz, 3H).

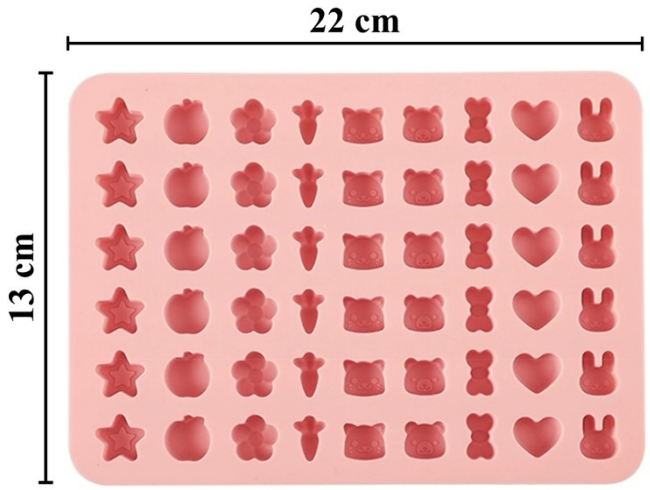


Figure S2 Photograph for silicone mold.

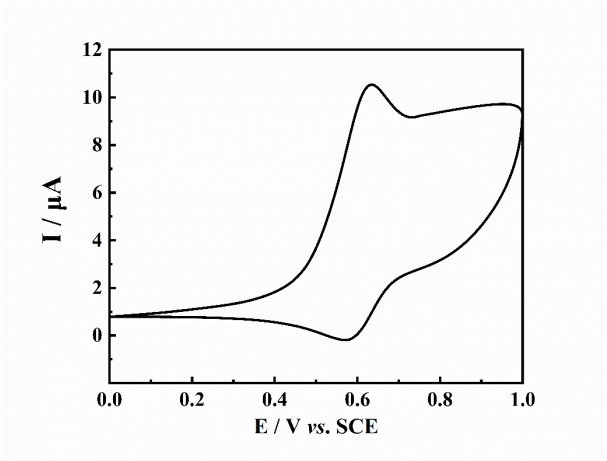


Figure S3 CV curve of FcMe-TPE in degassed DMF solution with a rate of 10 mV/s using Bu_4NPF_6 as electrolyte.

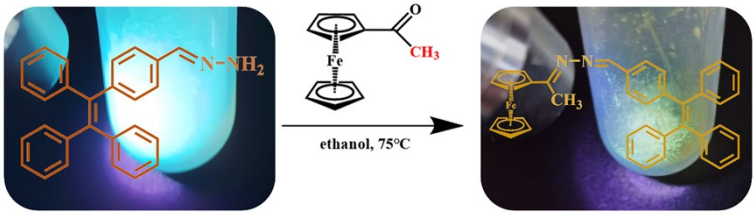


Figure S4 Illustration of fluorescence quenching phenomenon.

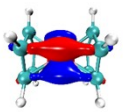
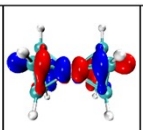
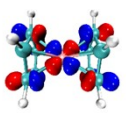
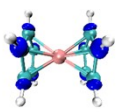
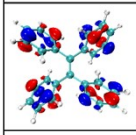
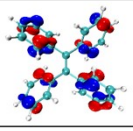
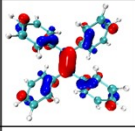
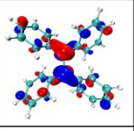
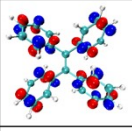
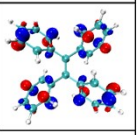
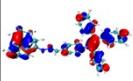
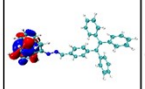
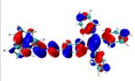
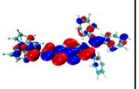
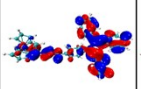
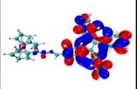
Fc						
	46a E = -0.2211 HOMO-2	47a E = -0.1903 HOMO-1	48a E = -0.1903 HOMO	49a E = -0.0093 LUMO	50a E = -0.0093 LUMO+1	51a E = 0.0552 LUMO+2
TPE						
	86a E = -0.2406 HOMO-2	87a E = -0.2370 HOMO-1	88a E = -0.1954 HOMO	89a E = -0.0442 LUMO	90a E = -0.0085 LUMO+1	91a E = -0.0079 LUMO+2
FcMe-TPE						
	151a E = -0.2248 HOMO-2	152a E = -0.2241 HOMO-1	153a E = -0.2171 HOMO	154a E = -0.0795 LUMO	155a E = -0.0508 LUMO+1	156a E = -0.0289 LUMO+2

Figure S5 HOMOs and LUMOs (HOMO, HOMO-1, HOMO-2, LUMO, LUMO+1 and LUMO+2) and energy levels of ferrocene groups, tetraphenylethene groups and FcMe-TPE.

The high symmetry of Fc resulting in its HOMO-1 was close in energy to HOMO and LUMO+1 was close in energy to LUMO. The electronic transitions for the FcMe-TPE were arranged in descending order of contribution and presented in Table S1. For FcMe-TPE, the absorption band mainly originated from HOMO-2 to LUMO electronic transition.

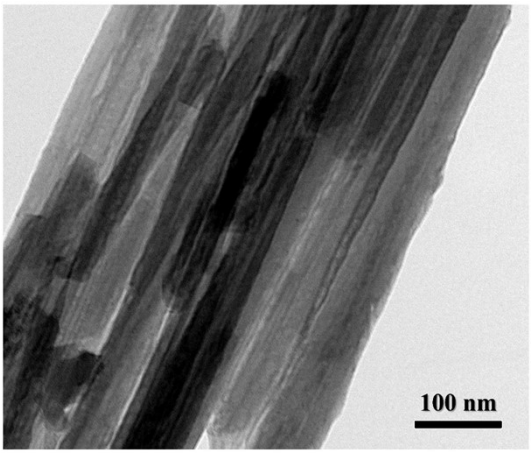


Figure S6 TEM image of PVA/FcMe-TPE hydrogel.

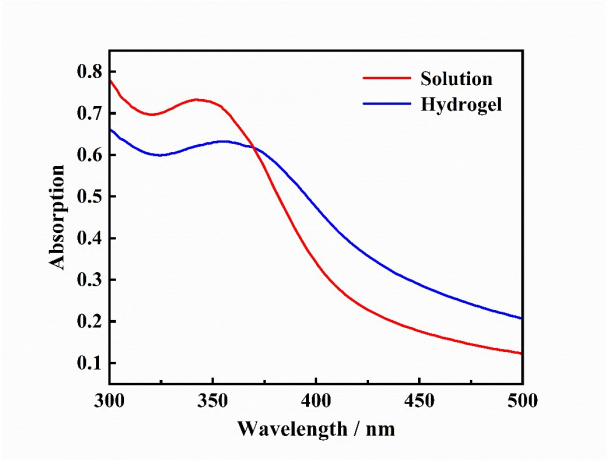


Figure S7 The UV-Vis absorption spectra of FcMe-TPE in solution and hydrogel.

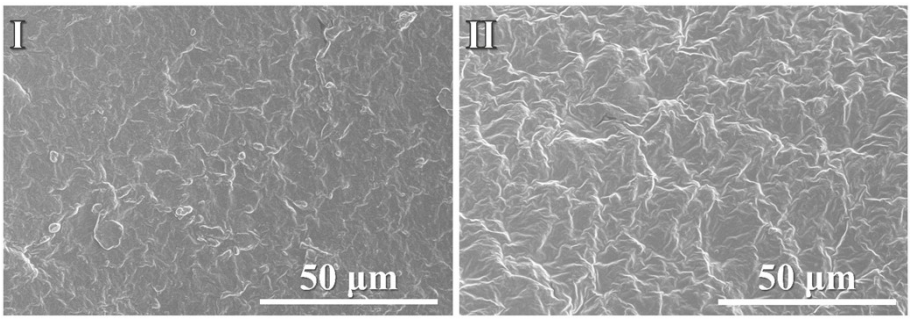


Figure S8 SEM images of PVA/FcMe-TPE + PA hydrogel: (I) surface and (II) sectional view.

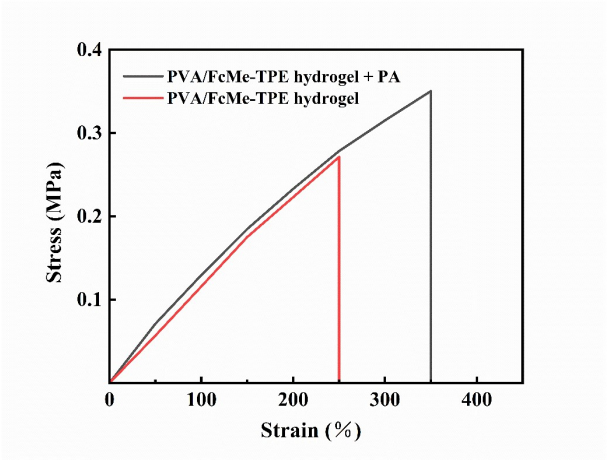


Figure S9 Stress-strain curve of PVA/FcMe-TPE hydrogel with/without PA.

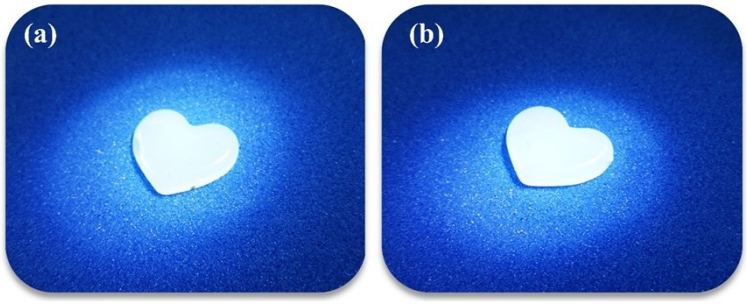


Figure S10 Optical images of hydrogel under UV light without PA (a) and with PA (b) after applying voltage.

Table S1 The contributions of orbital transition for FcMe-TPE in all excited states.

Excited state	Energy /eV	Wavelength /nm	Oscillator strength	Spin multiplicity	Major contribution
8	3.3855	366.22	0.00240	1	H-4 -> L 71.7%, H-5 -> L 13.9%, H-4 -> L+1 6.4%
9	3.5364	350.59	0.04910	1	H-2 -> L 43.4%, H-1 -> L+8 6.4%, H-2 -> L+10 5.6%, H -> L 5.4%
10	3.5717	347.13	0.00010	1	H-1 -> L 24.7%, H-5 -> L+8 18.0%, H-1 -> L+10 15.4%, H-1 -> L+9 9.1%, H -> L+8 6.8%, H-1 -> L+4 6.7%, H-2 -> L+8 6.4%, H-4 -> L+8 5.6%
11	3.8896	318.76	0.34560	1	H -> L+1 77.1%, H-2 -> L+1 18.7%