Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Exploring the Luminescence Properties and Sensing Mechanism of a Turn-on TADF Probe for Sulfite

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Table S1. The absorption properties for probe DCF-MPYM-lev and product DCF-MPYM calculated by several functionals.

Function	Molecule	States	Energy(eV)	Wavelength(nm)	Osciallor(a.u.)
B3lyp	DCF-MPYM-lev	S_4	3.11	399/370*	1.28
	DCF-MPYM	S_1	2.22	558/525*	0.26
		S_5	2.87	433/480*	0.64
M062x	DCF-MPYM-lev	S_2	3.65	340	2.09
	DCF-MPYM	S_1	2.80	443	0.73
		S_4	3.64	341	1.29
ωb_{97}xd	DCF-MPYM-lev	S_2	3.72	333	2.10
	DCF-MPYM	S_1	2.89	429	0.80
		S_4	3.71	335	1.34
Pbe0	DCF-MPYM-lev	S_2	3.72	333	2.10
	DCF-MPYM	S_1	2.89	429	0.80
		S_5	3.71	335	1.34

Table S2 Fluorescence properties, including the vertical excitation energies (E_{vt}/eV), radiative rates (k_r/s^{-1}), non-radiative decay rate (k_{nr}/s^{-1}), total reorganization energies (λ/cm^{-1}) and fluorescence efficiency ($\Phi/\%$) of DCF-MPYM and $[DCF-MPYM-2H]^{2-}$ with different conformers are calculated.

	E_{vt}	k_r	k_{nr}	λ	Φ
DCF-MPYM-A	1.54	3.57×10^7	2.23×10^9	3177	1.57%
DCF-MPYM-B	1.53	3.87×10^7	3.55×10^9	3190	1.08%
DCF-MPYM-C	1.54	2.93×10^7	2.03×10^{11}	4338	0.01%
A	1.94	4.28×10^7	3.44×10^8	936	11.04%
B	2.01	8.31×10^7	2.99×10^8	906	21.73%
C	1.90	452×10^7	3.56×10^8	1369	11.25%

Table S3 One-photon absorption properties including the excitation energy E_{opa} (eV), the corresponding wavelengths λ_{opa} (nm), the oscillator strengths δ_{opa} (a.u.) and transition nature of $DCF-MPYM-lev$ and $DCF-MPYM$.

Mol	Excited state	E_{opa}	λ_{opa}	δ_{opa}	Transition nature	
DCF-MPYM -lev	S4	3.11	399	1.28	H-1-L+1	41.6%
					H-1-L	26.9%
DCF-MPYM	S4	2.71	457	0.30	H-2-L	76.7%
	S5	2.87	433	0.64	H-L+2	65.6%

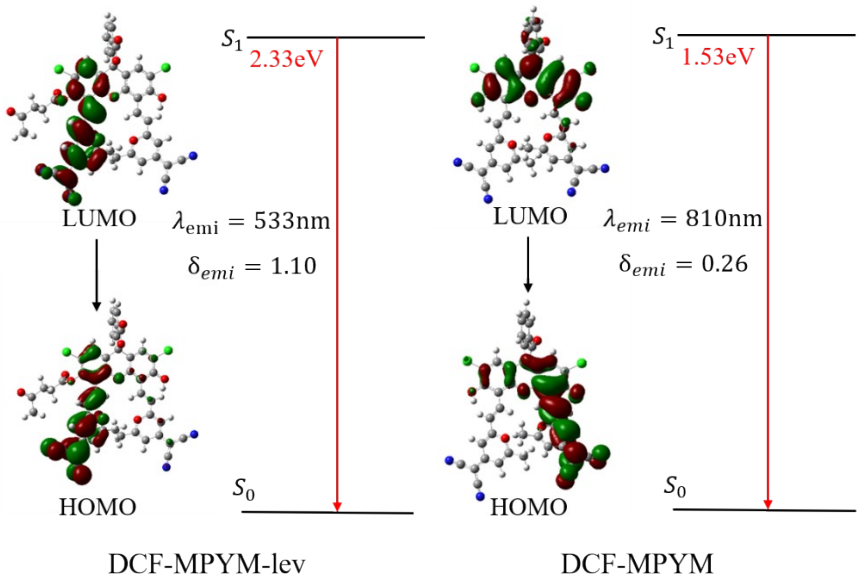

Figure S1. The emission properties of probe $DCF-MPYM-lev$ and $DCF-MPYM$. The green and red sections represent the positive and negative phases of the wave function respectively.

Table S4. Fluorescence properties, including the vertical excitation energies (E_{vt}/eV), radiative rates (k_r/s^{-1}), non-radiative decay rate (k_{nr}/s^{-1}), total reorganization energies (λ/cm^{-1}) and fluorescence efficiency ($\Phi/\%$) are calculated of $DCF-MPYM-lev$ and $DCF-MPYM$ with different conformers are calculated.

Mol	E_{vt}	k_r	k_{nr}	λ	Φ
DCF-MPYM-lev-B	2.33	3.22×10^8	7.22×10^7	2851	81.7%
DCF-MPYM-B	1.53	3.87×10^7	3.55×10^9	3190	1.08%

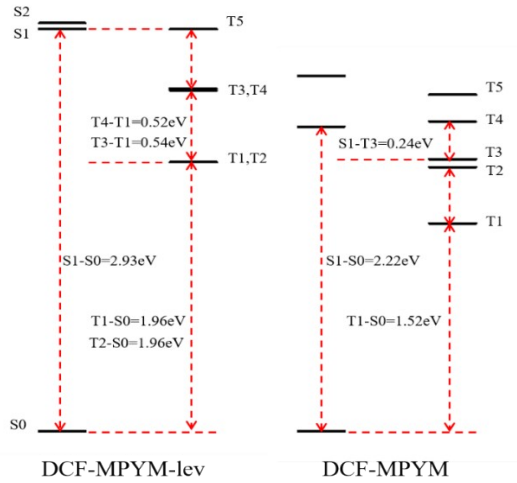

Figure S2. Excitation energies for $DCF-MPYM-lev$ and $DCF-MPYM$.

Table S5. Frontier energies (eV) of HOMO-3 to LUMO+3 for $[DCF-MPYM-lev-H]^-$ and $[DCF-MPYM-2H]^{2-}$ with different conformers in acetonitrile.

	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3
lev-A	-6.14	-5.98	-5.73	-4.94	-2.67	-2.22	-1.54	-1.43
lev-B	-6.13	-5.99	-5.70	-4.97	-2.70	-2.19	-1.57	-1.44
lev-C	-6.11	-5.99	-5.70	-4.92	-2.67	-2.19	-1.52	-1.43
A	-5.82	-5.55	-5.32	-4.96	-2.30	-2.24	-1.95	-1.17
B	-5.82	-5.54	-5.32	-4.98	-2.28	-2.24	-1.96	-1.14
C	-5.81	-5.53	-5.27	-4.95	-2.33	-2.21	-1.94	-1.20

Figure S3. The orbitals distribution form HOMO-3 to LUMO+3 of probe $DCF-MPYM-lev$ and $DCF-MPYM$.