

Supplementary Material

Modulating the ESIPT Mechanism and Luminescence Characteristics of Two Reversible Fluorescent Probes by Solvent Polarity: A Novel Perspective

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Table S1. Bond length (Å), bond angles and dihedral angles (°) of HTP-1 and HTP-2 in different electron states.

			O ₁ -H ₁	N ₁ -H ₁	δ(O ₁ -H ₁ -N ₁)	C ₅ -C ₁ -C ₂ -C ₃	C ₁ -C ₂ -C ₃ -C ₄	C ₂ -C ₁ -C ₅ -C ₆	C ₂ -C ₁ -C ₇ -C ₈	C ₁ -C ₂ -C ₉ -C ₁₀
HTP-1	ACN	S ₀	0.997	1.707	147.79	12.35	48.40	47.66	47.34	47.62
		S ₁	0.997	1.709	148.12	58.67	17.02	21.07	24.06	28.03
	ACE	S ₀	0.997	1.708	147.74	12.34	48.37	47.64	47.28	47.56
		S ₁	0.997	1.711	148.07	53.66	18.37	21.59	25.17	27.97
	DCM	S ₀	0.997	1.711	147.63	12.32	48.30	47.58	47.09	47.41
		S ₁	0.996	1.714	147.94	52.75	18.63	21.63	25.33	27.85
	n-Hexane	S ₀	0.995	1.726	147.08	12.24	48.15	47.13	46.60	46.89
		S ₁	0.994	1.727	147.34	50.21	19.12	21.15	25.86	27.45
	ACN	S ₀	0.990	1.775	145.68	12.56	47.76	47.54	47.31	47.53
		S ₁	0.999	1.687	146.60	20.22	38.45	40.82	40.72	43.38
HTP-2	ACN	S ₁ '	1.881	1.026	126.13	12.63	48.98	48.54	46.39	46.40
		S ₀	0.990	1.776	145.64	12.53	47.82	47.45	47.26	47.49
	ACE	S ₁	1.000	1.685	146.63	20.24	38.42	40.79	40.65	43.29
		S ₁ '	2.010	1.022	120.44	9.69	50.46	47.09	47.22	46.04
	DCM	S ₀	0.989	1.778	145.54	12.46	47.92	47.26	47.12	47.41
		S ₁	1.000	1.682	146.71	20.32	38.35	40.66	40.48	43.10
	n-Hexane	S ₁ '	1.981	1.023	121.90	9.63	50.93	47.14	46.96	45.74
		S ₀	0.988	1.789	145.10	12.23	47.75	46.87	46.63	47.29
	n-Hexane	S ₁	1.003	1.660	147.13	20.75	38.29	40.16	39.97	42.35
		S ₁ '	1.886	1.027	126.50	9.90	52.01	47.31	45.92	44.83

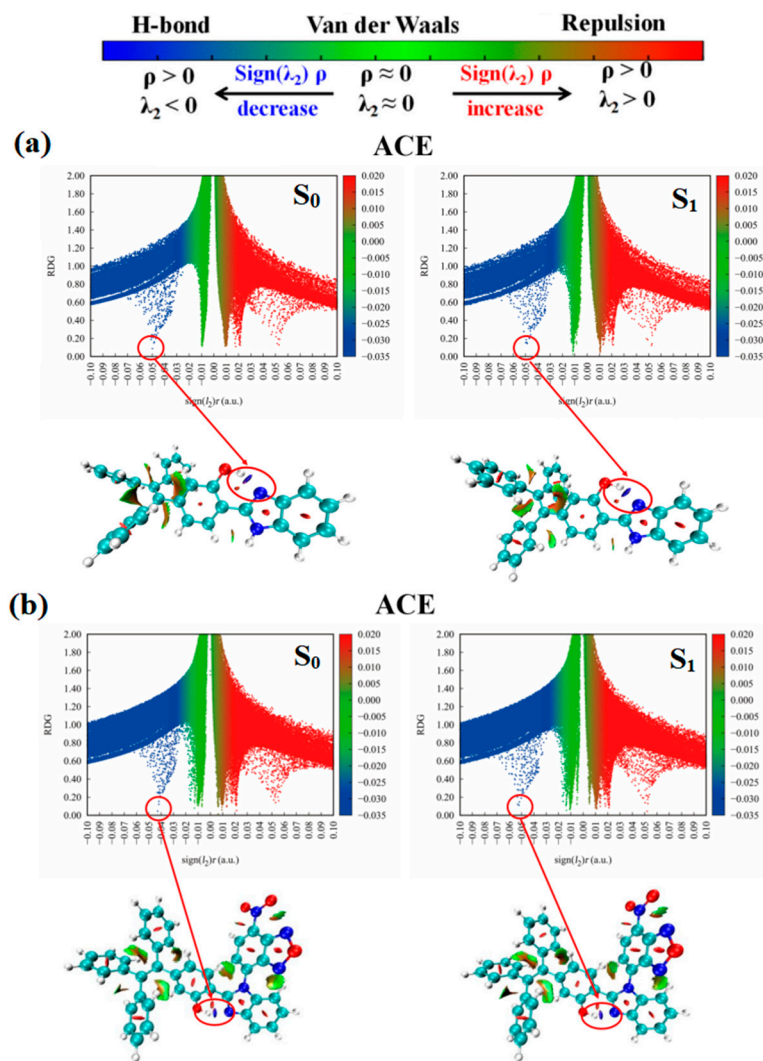


Figure S1. Reduced density gradient (RDG) versus $X(r)$ scatter plots in ACE: (a) HTP-1, (b) HTP-2.

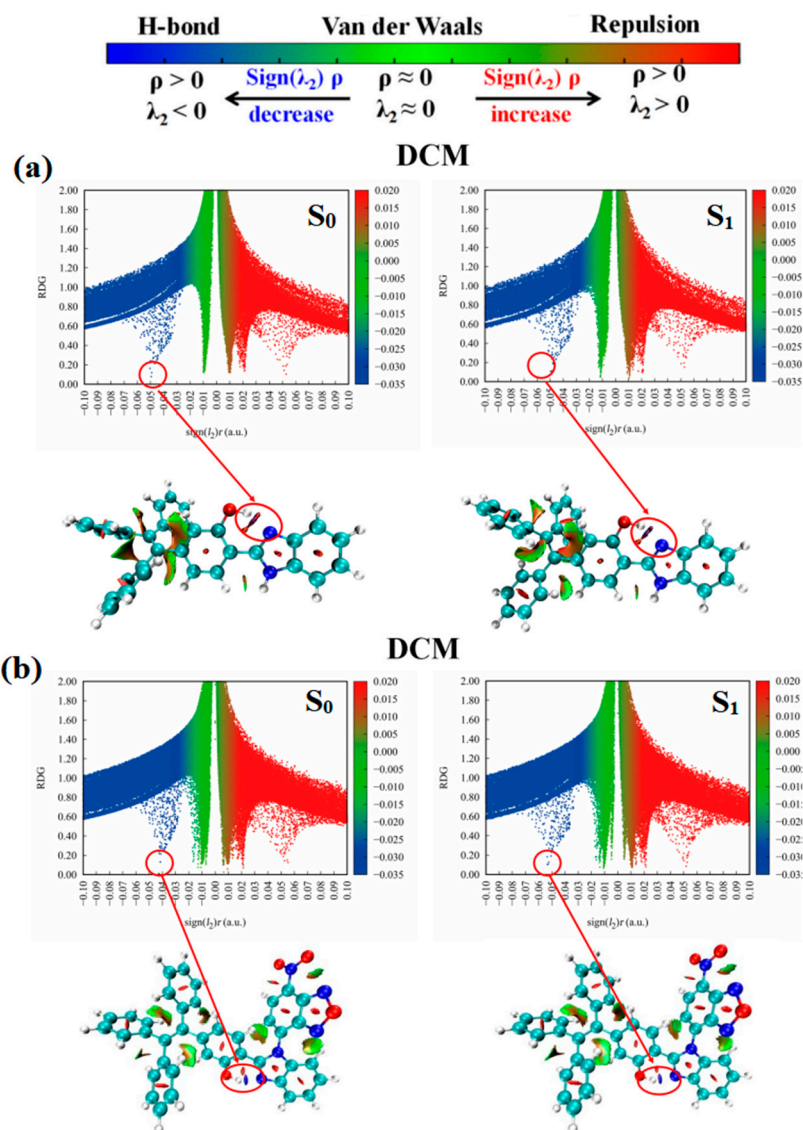


Figure S2. Reduced density gradient (RDG) versus $X(r)$ scatter plots in DCM: (a) HTP-1, (b) HTP-2.

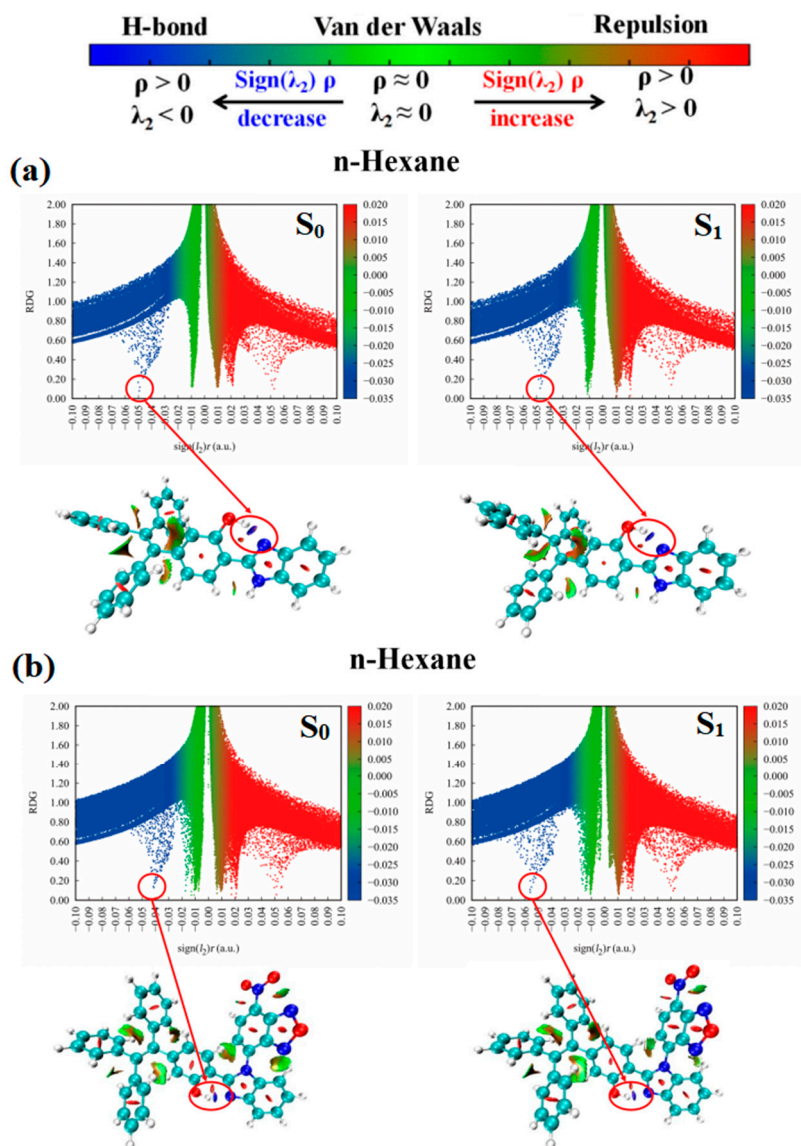


Figure S3. Reduced density gradient (RDG) versus $X(r)$ scatter plots in n-Hexane: (a) HTP-1, (b) HTP-2.

Table S2. Dielectric constant and polarity of four solvents.

Solvents	Dielectric constant	Polarity
ACN	37.5	6.2
ACE	20.7	5.4
DCM	9.08	3.4
n-Hexane	1.58	0.06

Table S3. The experimental and theoretical data of absorption and emission spectra of HTP-1 and HTP-2 in four solvents.

		Exp.	Theor.
HTP-1	ACN	348	351
	DCM	360	352
	n-Hexane	345	352