Supporting information for:

Aggregation-induced emission enhancement and mechanofluorochromic of α-cyanostilbene functionalized tetraphenyl imidazole derivatives

Yuyang Zhang[a], Huifang Li[a], Gaobin Zhang[a], Xianyun Xu[a], Lin Kong*[a], Xutang Tao[b], Yupeng Tian[a] and Jiaxiang Yang*[a,b]

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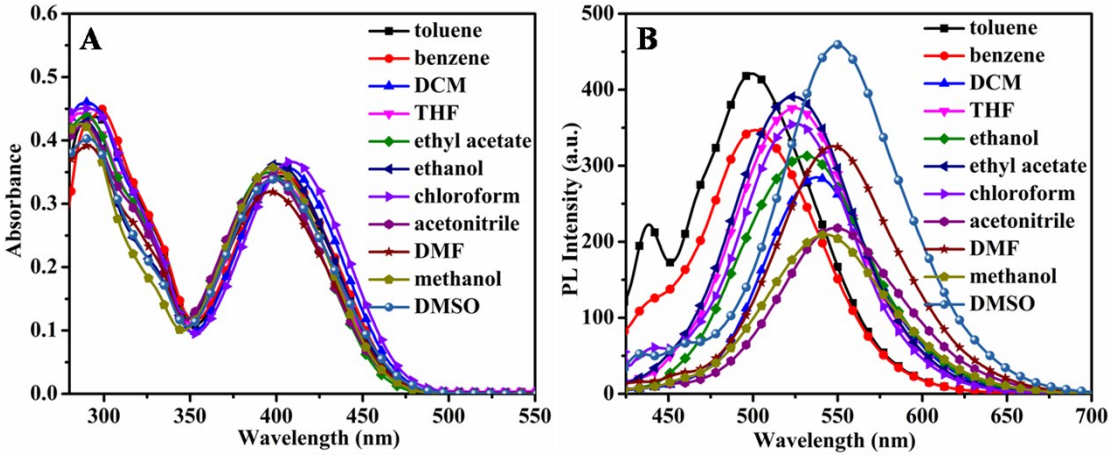

Fig. S1 The UV-vis spectra (A) and fluorescence spectra (B) of compound **3b** in different solvents (1×10^{-5} mol·L^{-1}).

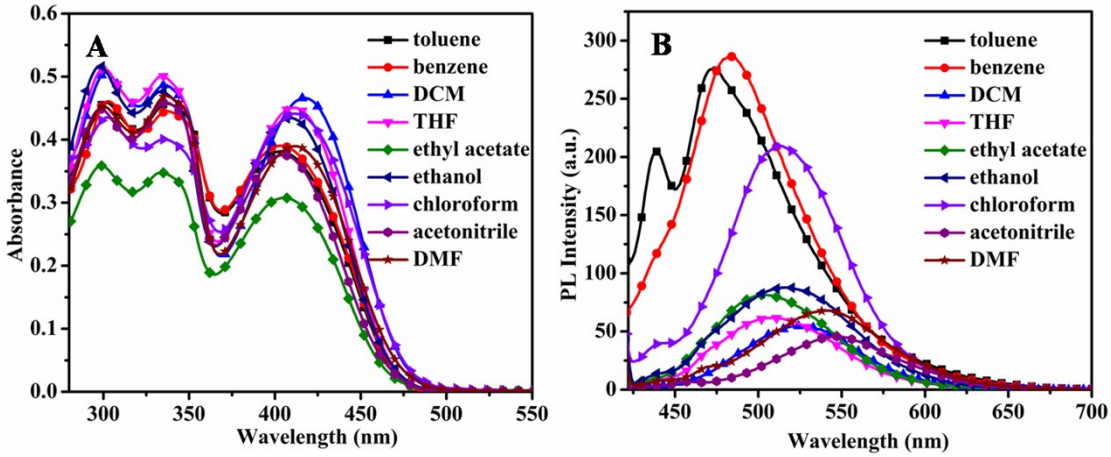

Fig. S2 The UV-vis spectra (A) and fluorescence spectra (B) of compound **3c** in different solvents (1×10^{-5} mol·L^{-1}).

Table S1 Photophysical properties of compounds **3a-3c** in different polar solvents

Compounds	Solvents	λ[a] max	λ[b] max	ε ($\times 10^4$)[c]	Δν [d]	Φ[e]
	toluene	395	481	5.12	4526	
	benzene	395	489	5.50	4866	
	DCM	413	520	4.77	4982	
	THF	409	507	5.23	4726	
3a	ethyl acetate	400	505	4.71	5198	0.11
	ethanol	405	520	3.44	5460	
	chloroform	407	509	4.74	4923	
	acetonitrile	402	544	5.40	6493	
	DMF	411	538	4.91	5743	
	toluene	401	499	3.44	4897	
	benzene	403	500	3.49	4813	
	DCM	405	538	3.58	6103	
	THF	400	525	3.41	5952	
	ethyl acetate	395	523	3.50	6195	
3b	ethanol	400	531	3.63	6167	0.37
	chloroform	409	526	3.67	5438	
	acetonitrile	395	548	3.43	7068	
	DMF	397	547	3.19	6907	
	methanol	398	543	3.57	6709	
	DMSO	399	550	3.39	6880	
	toluene	404	473	3.82	3610	
	benzene	404	484	3.91	4091	
	DCM	416	524	4.66	4954	
	THF	412	508	4.51	4586	
3c	ethyl acetate	405	503	3.08	4810	0.15
	ethanol	410	516	4.35	5010	
	chloroform	412	512	4.42	4740	
	acetonitrile	405	548	3.76	6443	
	DMF	412	542	3.90	5821	

[a] Peak position of the longest absorption band. [b] Peak position of fluorescence emission, excited at the absorption maximum. [c] Molar absorptivity (L/cm/mol). [d] Stokes' shift in cm^{-1}. [e] Quantum yields in solid state.

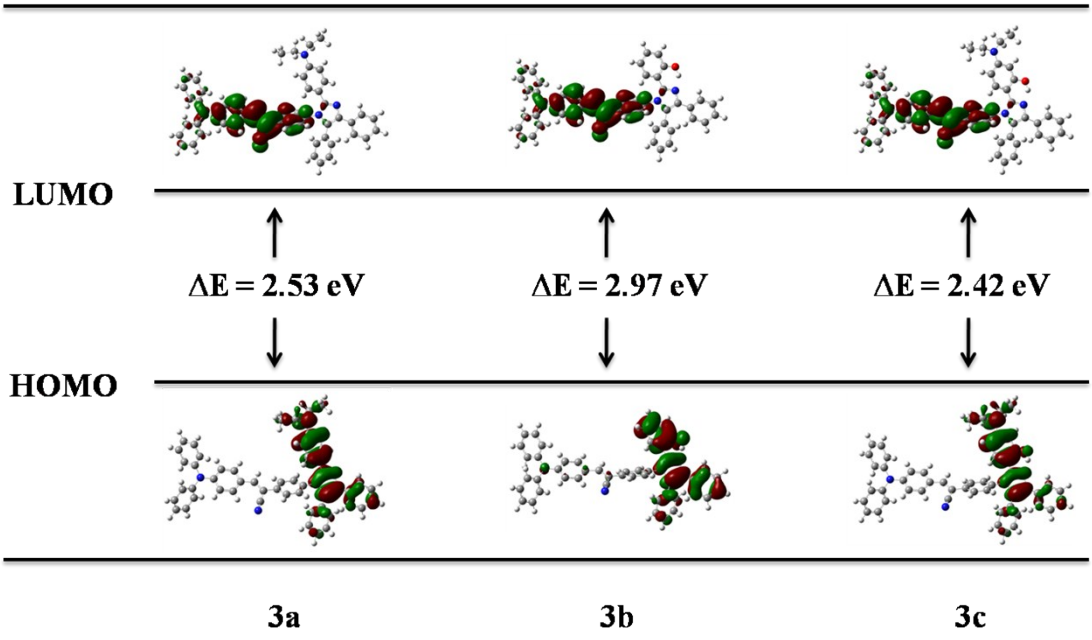

Fig. S3 Optimized molecular structures and molecular orbital amplitude plots of the HOMO and LUMO levels, energy gaps and electron cloud distribution of **3a**, **3b** and **3c** calculated using the B3LYP/6-31G* basis set.

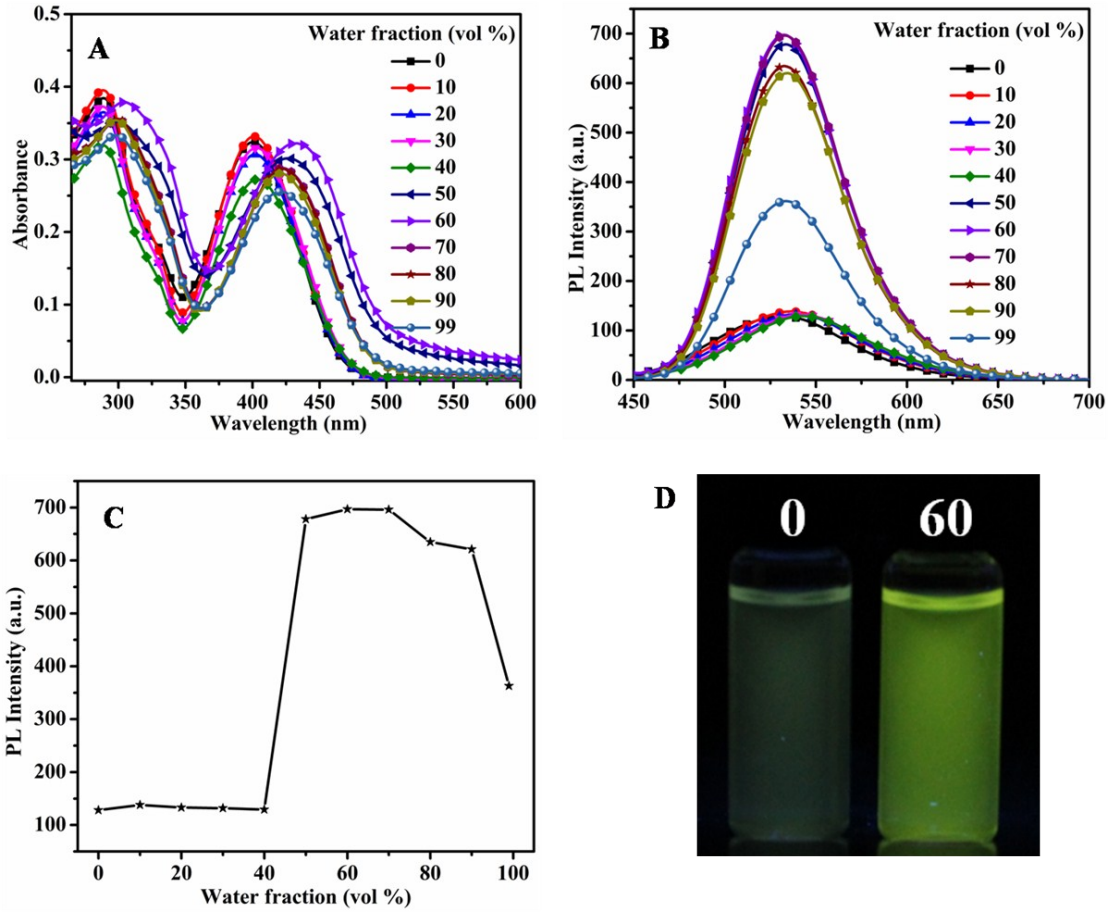

Fig. S4 The UV-vis absorption (A) and fluorescence spectra of compound **3b** in ethanol-water mixtures with different water volume fractions; the effect of water volume fraction on the maximum emission intensity (C); optical photographs recorded under 365 nm UV irradiation with various fractions of water (D).

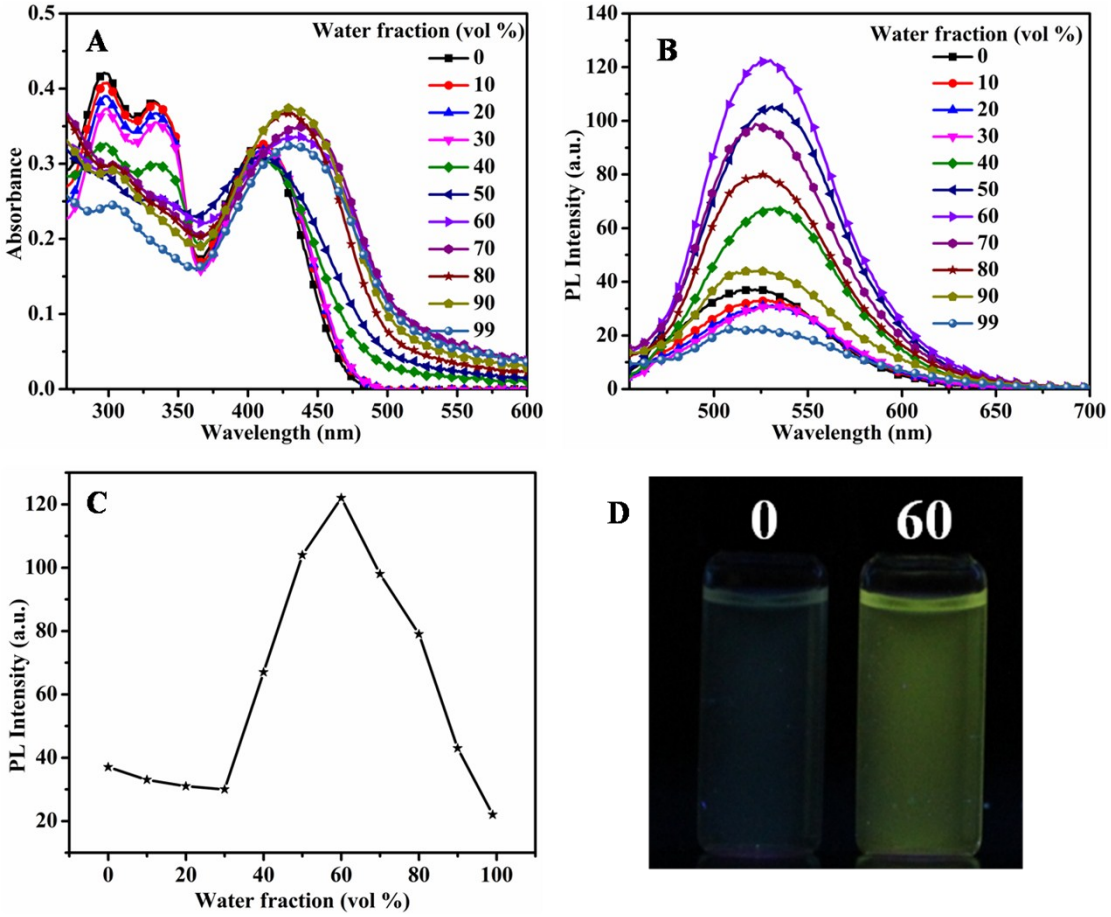

Fig. S5 The UV-vis absorption (A) and fluorescence spectra of compound **3c** in ethanol-water mixtures with different water volume fractions; the effect of water volume fraction on the maximum emission intensity (C); optical photographs recorded under 365 nm UV irradiation with various fractions of water (D).

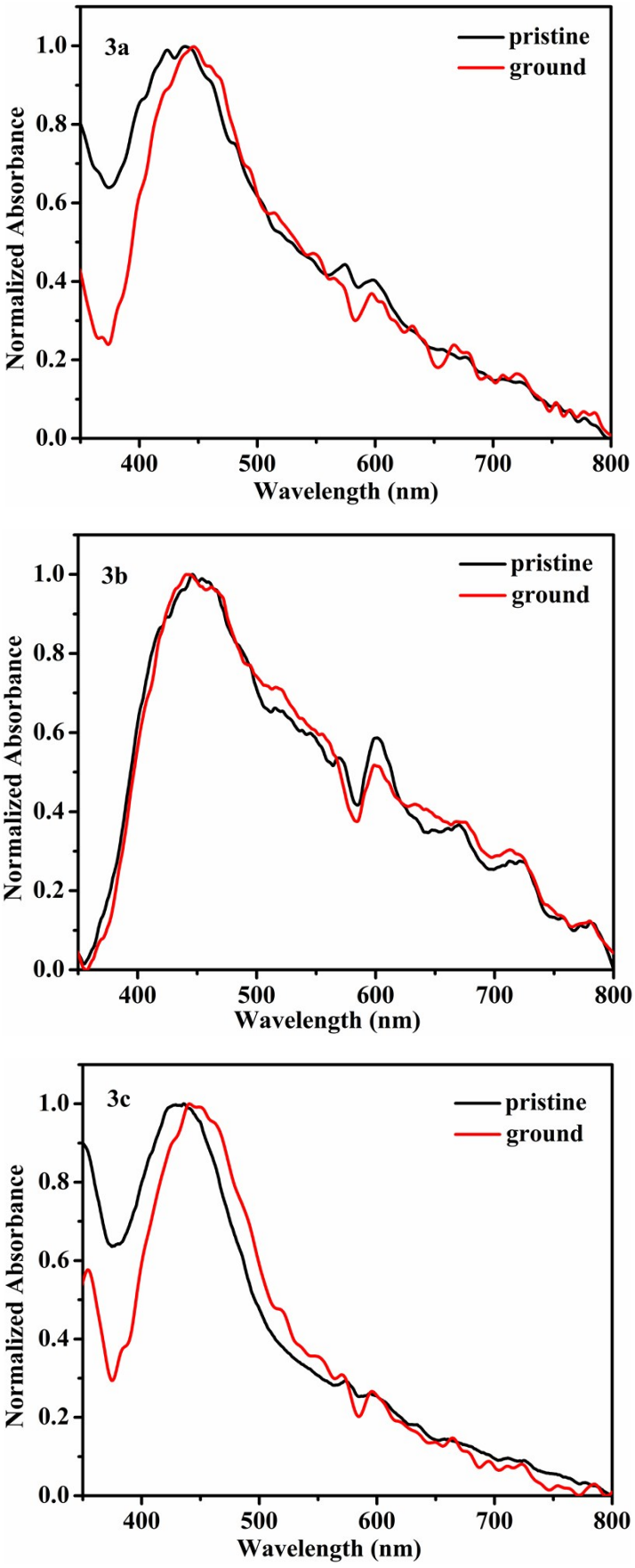

Fig. S6 Normalized UV-vis absorption spectra of **3a-3c** solids under different conditions.

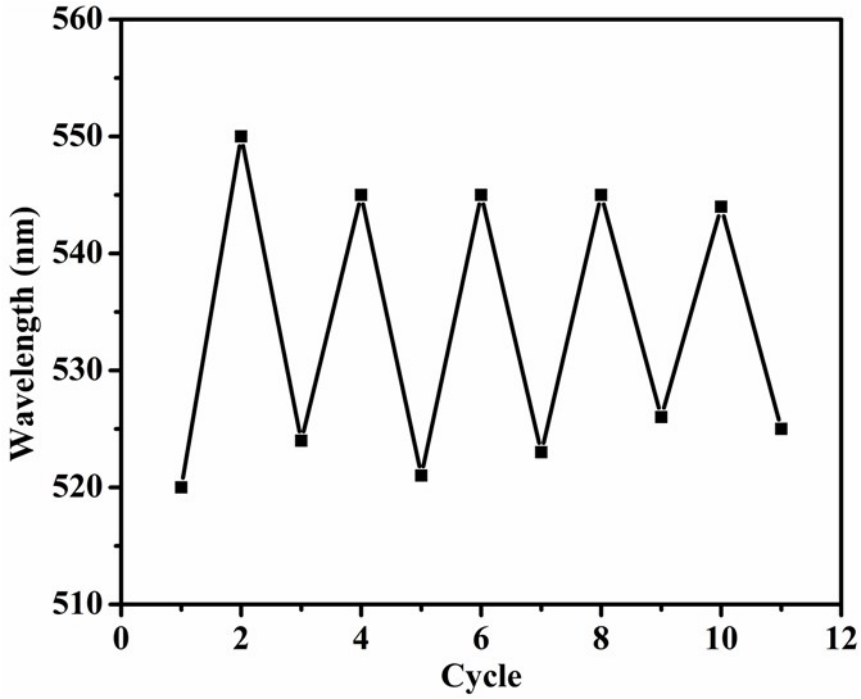

Fig.S7 Repeated switching of compound **3a** between green and yellow emission by ground-fumed cycles.

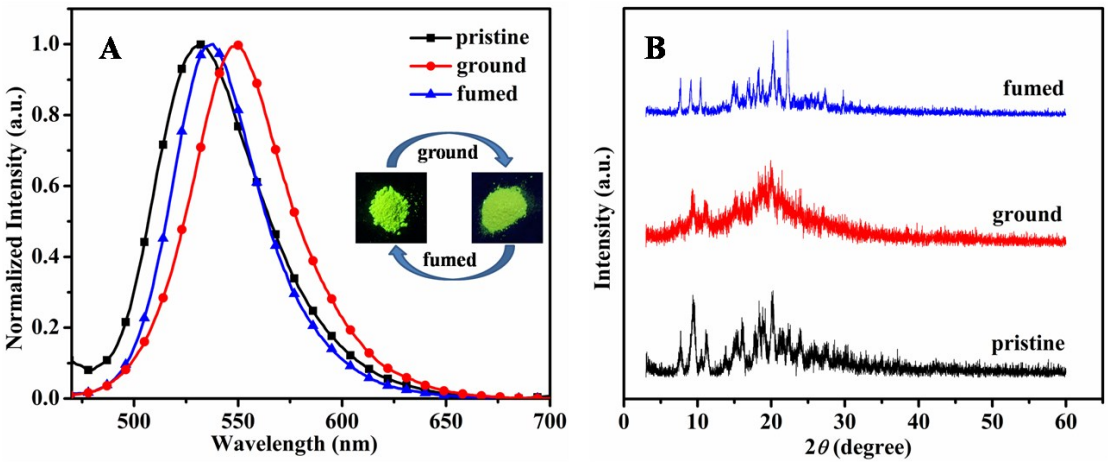

Fig. S8 Emission spectra (A) and XRD patterns (B) of pristine, ground and fumed with ethanol of compound **3b**. Inset: photographs of pristine and ground powders under 365 nm light.

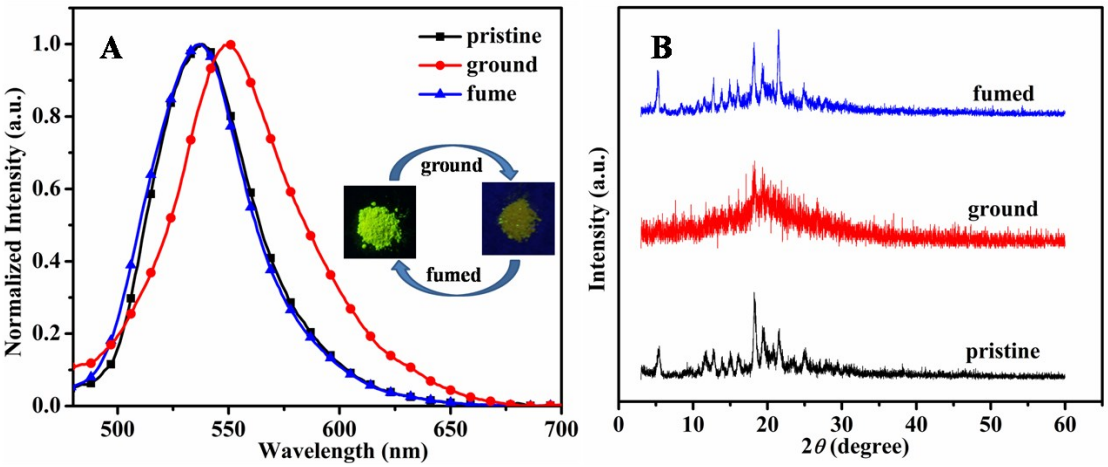

Fig. S9 Emission spectra (A) and XRD patterns (B) of pristine, ground and fumed with ethanol of compound **3c**. Inset: photographs of pristine and ground powders under 365 nm light.

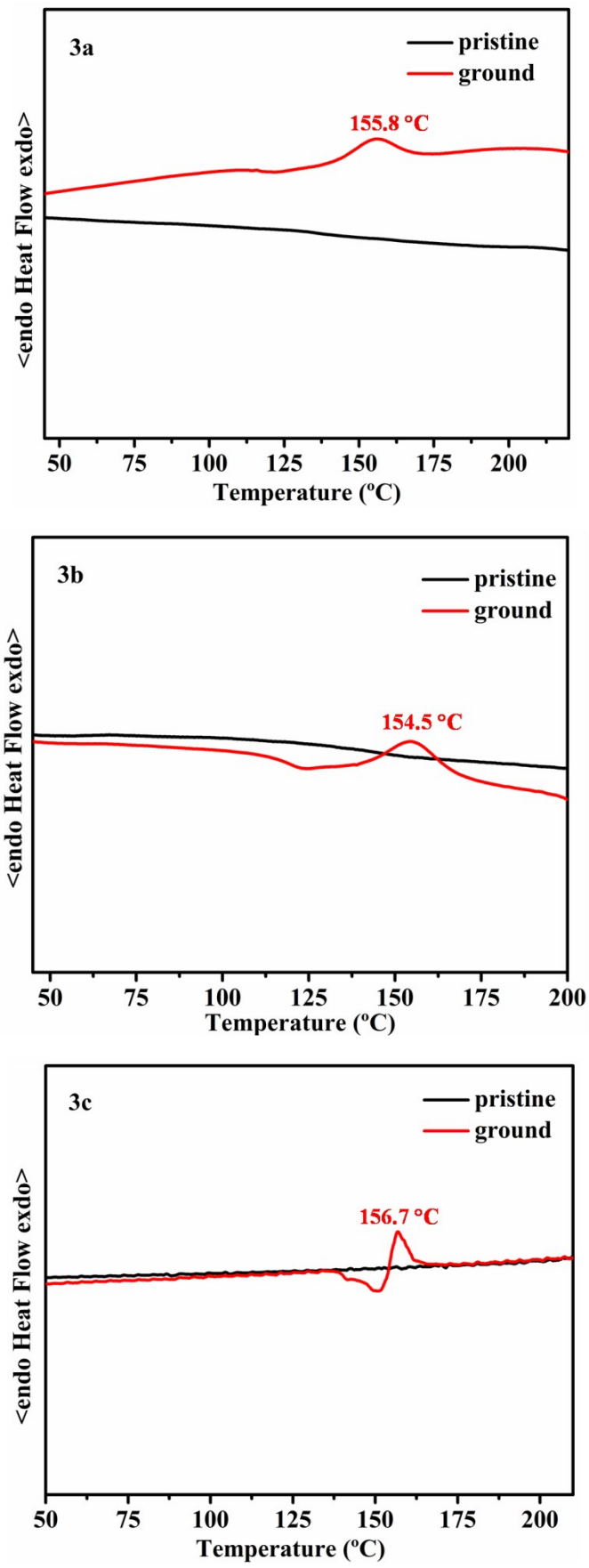

Fig. S10 DSC curves of **3a-3c** in the pristine and ground powders. (scan rate: 10 °C min^{-1})

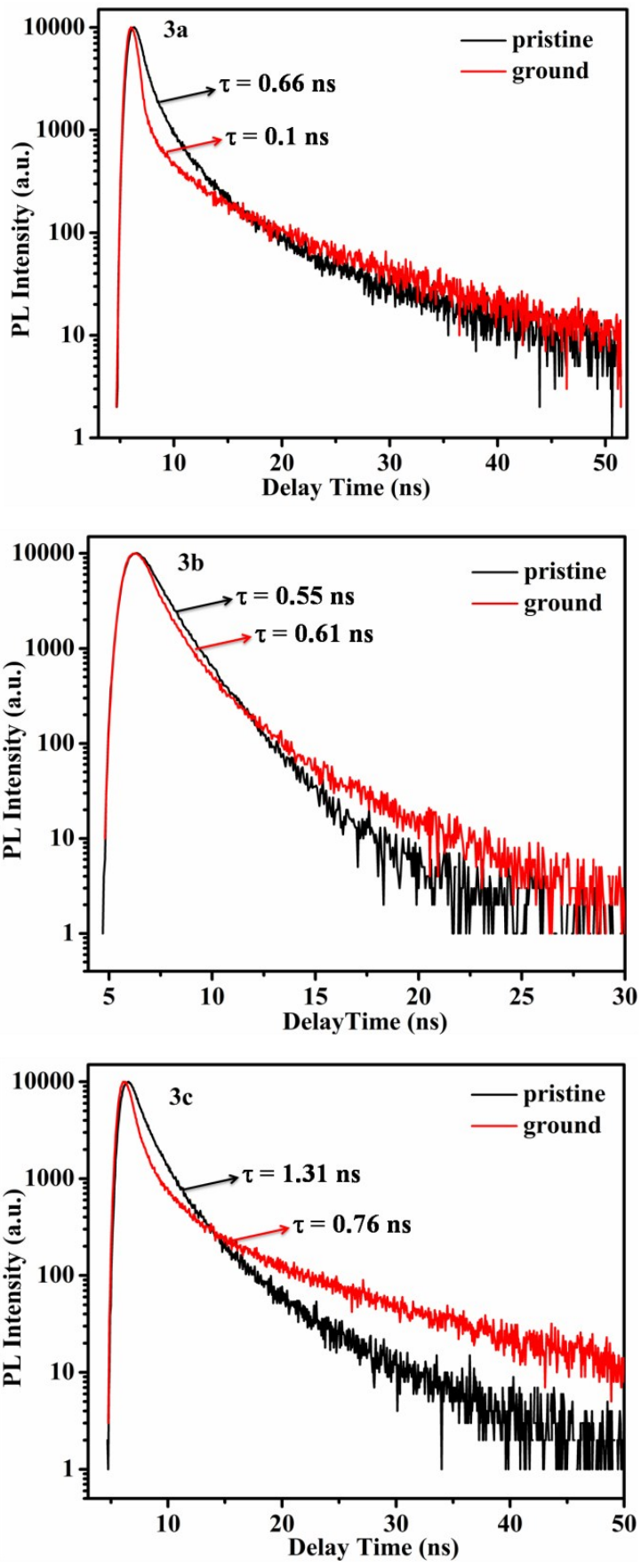

Fig. S11 Fluorescence emission decay lifetime of **3a**, **3b** and **3c** at pristine and ground state.

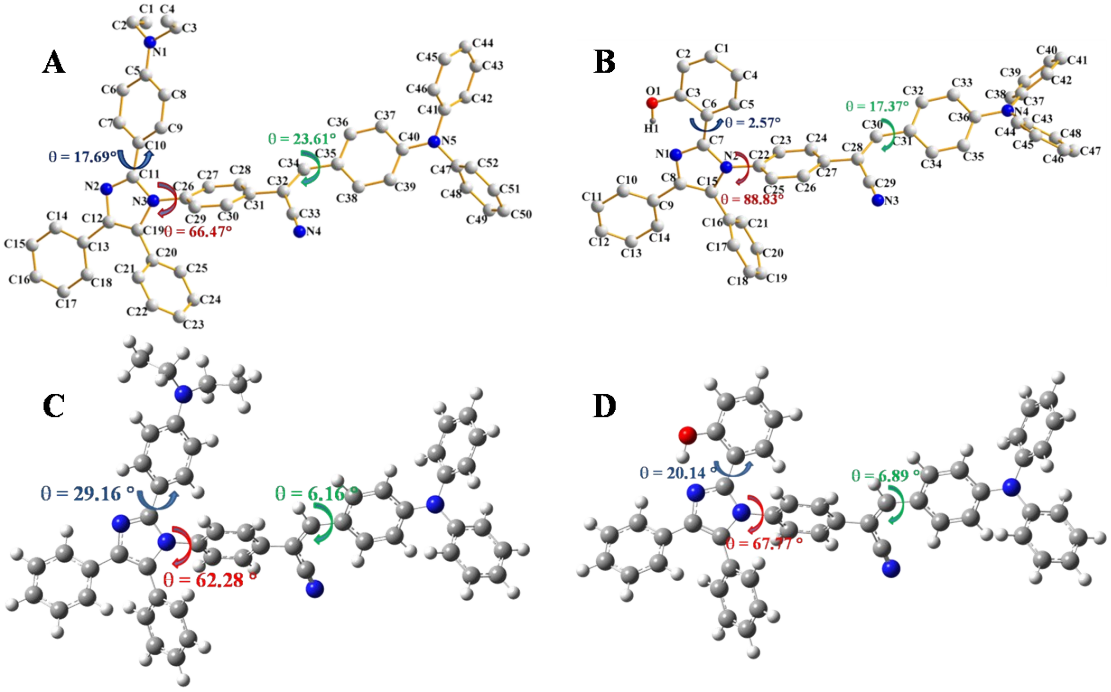

Fig. S12 Crystal structures (A and B) and optimization geometry structures (C and D) of compounds **3a** and **3b**

Table S2 Selected bond distances (Å) and bond angles (°) for compound **3a**

N(3)-C(11)	1.382(4)	C(11)-N(3)-C(19)	107.7(3)
N(3)-C(19)	1.404(4)	C(11)-N(3)-C(26)	127.9(3)
N(3)-C(26)	1.440(4)	C(19)-N(3)-C(26)	123.9(3)
N(2)-C(11)	1.317(4)	N(2)-C(11)-N(3)	110.4(3)
N(2)-C(12)	1.392(4)	N(2)-C(11)-C(10)	123.0(3)
C(11)-C(10)	1.465(4)	C(19)-C(12)-N(2)	110.1(3)
C(12)-C(19)	1.379(4)	C(19)-C(12)-C(13)	131.2(3)
C(12)-C(13)	1.483(5)	N(2)-C(12)-C(13)	118.5(3)
C(19)-C(20)	1.480(4)	C(12)-C(19)-N(3)	104.8(3)
C(34)-C(32)	1.349(4)	N(3)-C(19)-C(20)	121.2(3)
C(32)-C(33)	1.431(5)	C(34)-C(32)-C(33)	121.7(3)
C(5)-N(1)	1.384(4)	C(34)-C(32)-C(31)	123.4(3)
N(5)-C(40)	1.391(4)	C(33)-C(32)-C(31)	114.9(3)
N(5)-C(41)	1.441(4)	N(4)-C(33)-C(32)	177.8(4)

Table S3 Hydrogen-bonding geometry of compound **3a** (bond distances [Å] and bond angles [°])

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*
C43-H43···N2	0.93	2.74	3.63	160

Table S4 Selected bond distances (Å) and bond angles (°) for compound **3b**

O(1)-C(3)	1.350(5)	C(7)-N(1)-C(8)	108.7(3)
N(1)-C(7)	1.331(5)	C(15)-N(2)-C(7)	107.7(3)
N(1)-C(8)	1.377(5)	C(15)-N(2)-C(22)	124.3(3)
N(2)-C(15)	1.388(5)	C(7)-N(2)-C(22)	127.9(4)
N(2)-C(7)	1.391(5)	N(1)-C(8)-C(15)	108.6(4)
N(2)-C(22)	1.430(5)	N(1)-C(8)-C(9)	120.4(4)
C(8)-C(15)	1.380(5)	N(1)-C(7)-N(2)	108.6(4)
C(8)-C(9)	1.472(6)	N(1)-C(7)-C(6)	122.8(4)
C(7)-C(6)	1.456(6)	N(2)-C(7)-C(6)	128.6(4)
C(15)-C(16)	1.472(6)	C(8)-C(15)-N(2)	106.4(4)
C(29)-C(28)	1.437(6)	N(3)-C(29)-C(28)	177.7(5)
C(30)-C(28)	1.337(6)	C(28)-C(30)-C(31)	131.7(4)
N(4)-C(36)	1.416(5)	C(30)-C(28)-C(29)	121.7(4)
N(4)-C(43)	1.428(5)	C(29)-C(28)-C(27)	115.0(4)
N(4)-C(37)	1.428(5)	O(1)-C(3)-C(2)	117.1(4)
N(3)-C(29)	1.146(5)	O(1)-C(3)-C(6)	122.3(5)

Table S5 Hydrogen-bonding geometry of compound **3b** (bond distances [Å] and bond angles [°])

D-H···*A*	*D*-H	*H*···*A*	*D*···*A*	*D*-H···*A*
O1-H1···N1	0.82	1.81	2.55	149