Electronic Supplementary Information

Polymorphic and Mechanochromic Luminescence Modulation in the Highly Emissive Dicyanodistyrylbenzene Crystal: Secondary Bonding Interaction in Molecular Stacking Assembly

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Complete reference

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Table S1. Crystallographic data of BDCS phase **I** single crystal.

Identification code	bdcs	
Empirical formula	C24H16 N2	
Formula weight	332.38	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 6.8239(4) Å	α= 90°.
	b = 7.2324(3) Å	β= 90°.
	c = 35.2082(15) Å	γ = 90°.
Volume	1737.64(15) $Å^3$	
Z	4	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	696	
Crystal size	0.33 x 0.24 x 0.08 mm^3	
Theta range for data collection	1.16 to 27.50°.	
Index ranges	-8<=h<=8, -9<=k<=7, -45<=l<=35	
Reflections collected	8242	
Independent reflections	1989 [R(int) = 0.0374]	
Completeness to theta = 27.50°	99.7 %	
Absorption correction	None	
Max. and min. transmission	0.9944 and 0.9757	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1989 / 0 / 118	
Goodness-of-fit on F^2	1.140	
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1318	
R indices (all data)	R1 = 0.0665, wR2 = 0.1538	
Largest diff. peak and hole	0.179 and -0.224 $e.Å^{-3}$	

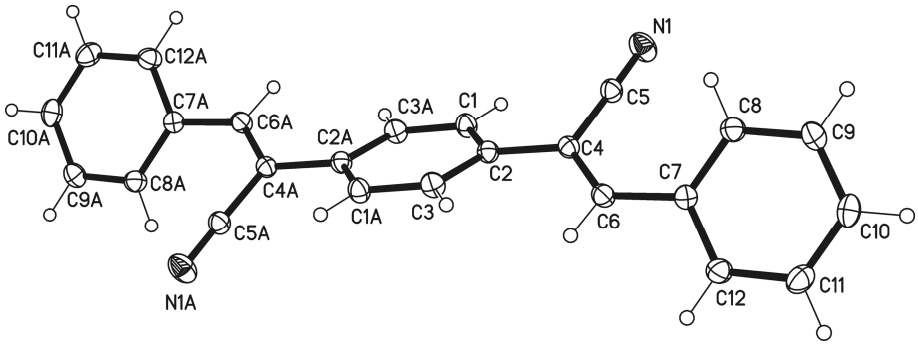

Fig. S1 ORTEP drawing of BDCS single crystal.

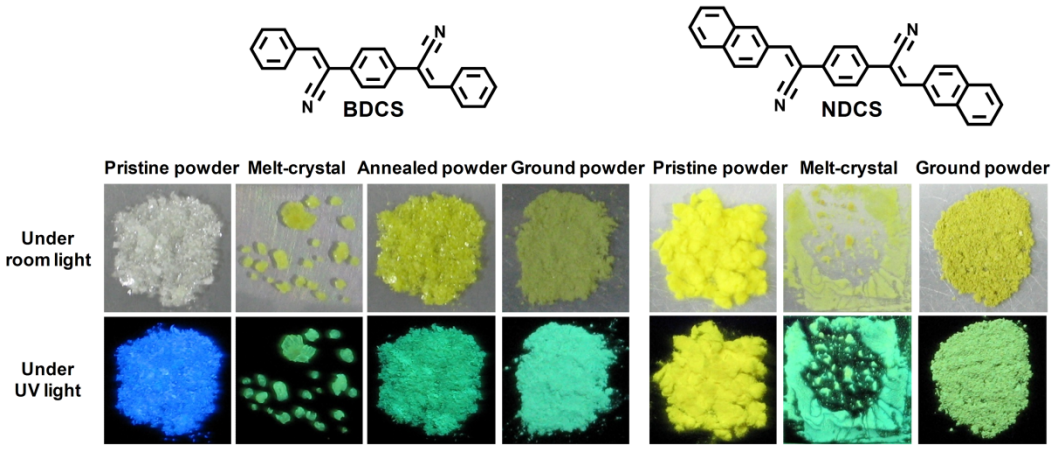

Fig. S2 BDCS and NDCS powders under various treatment conditions.

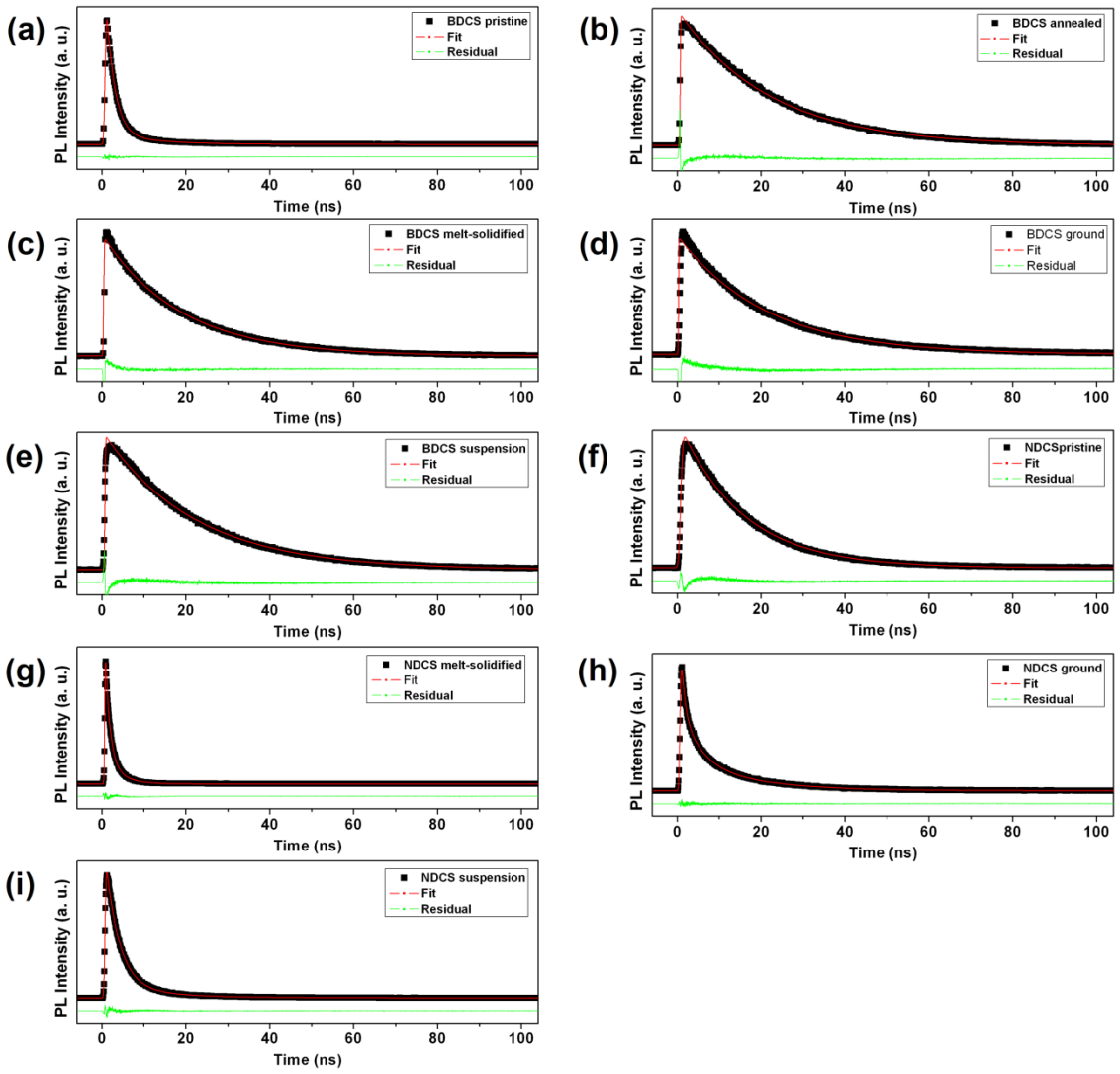

Fig. S3 Fluorescence decay profiles (black lines), fitting curves (red lines), residuals (green lines): (a) BDCS pristine powder. (b) BDCS annealed powder. (c) BDCS melt-solidified powder. (d) BDCS ground powder. (e) BDCS suspension. (f) NDCS pristine powder. (g) NDCS melt-solidified powder. (h) NDCS ground powder. (i) NDCS suspension.

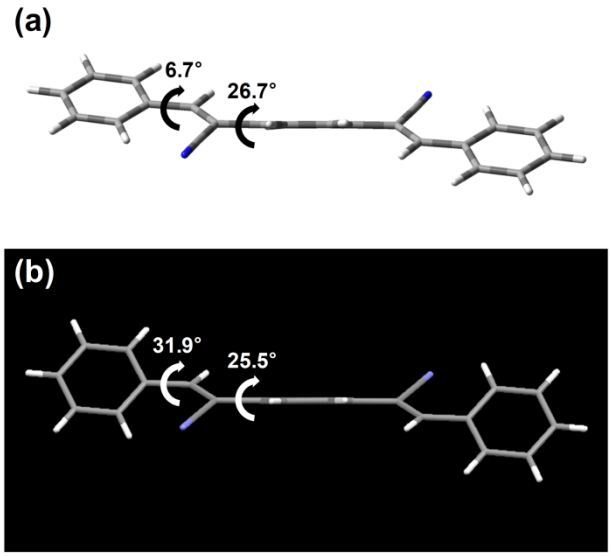

Fig. S4 (a) The calculated optimized geometry of the isolated BDCS. (b) The geometry of BDCS in the single crystal phase on the basis of results from the single crystal X-ray analysis.