Electronic Supplementary Information

Polymorphism-dependent fluorescence of bisthienylmaleimide with different responses to mechanical crushing and grinding pressure

Zhenghuan Lin, Xiaofei Mei, E Yang, Xiaoju Li, Huimei Yao, Guixiu Wen, Ching-Ting Chien, Tahsin J. Chow* and Qidan Ling*

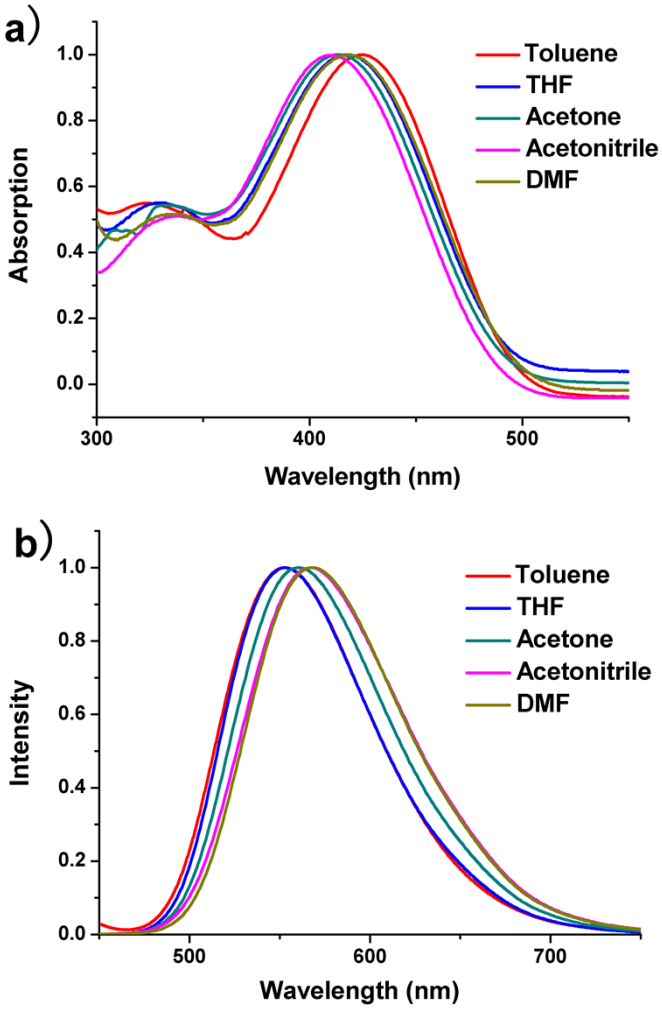

Fig. S1 Solvent effect: a) The absorption spectra of BTM in various solvents; b) The emission spectra of BTM in various solvents upon irradiation at λ_{max} of their absorption bands.

Table S1 The absorption and emission wavelength of BTM in several solvents

	λ_{abs}, nm	λ_{em}, nm
Toluene	325, 425	553
THF	330, 418	552
Actetone	331, 414	561
Acetonitrile	334, 411	567
DMF	335, 418	568

Table S2 Calculated wavelength (λ) and oscillator strength (f) for absorption and emission of BTM.

		Main orbital transition[a] (CIC)	λ[b], nm	f
Absorption	$S_0 \rightarrow S_1$	HOMO→LUMO (0.62)	481	0.2380
	$S_0 \rightarrow S_2$	HOMO-4→LUMO (-0.40) HOMO-1→LUMO (0.58)	381	0.0067
	$S_0 \rightarrow S_3$	HOMO-3→LUMO (-0.38) HOMO-2→LUMO (0.59)	347	0.0000
Emission	$S_1 \rightarrow S_0$	LUMO→HOMO (0.59)	602	0.1839
	$S_2 \rightarrow S_0$	LUMO→HOMO-4 (-0.48) LUMO→HOMO-1 (0.51)	405	0.0131
	$S_3 \rightarrow S_0$	LUMO→HOMO-4 (-0.51) LUMO→HOMO-1 (-0.49)	372	0.0096

[a] CI expansion coefficients for the main orbital transitions. [b] The data in parentheses is the experimental value in THF solution.

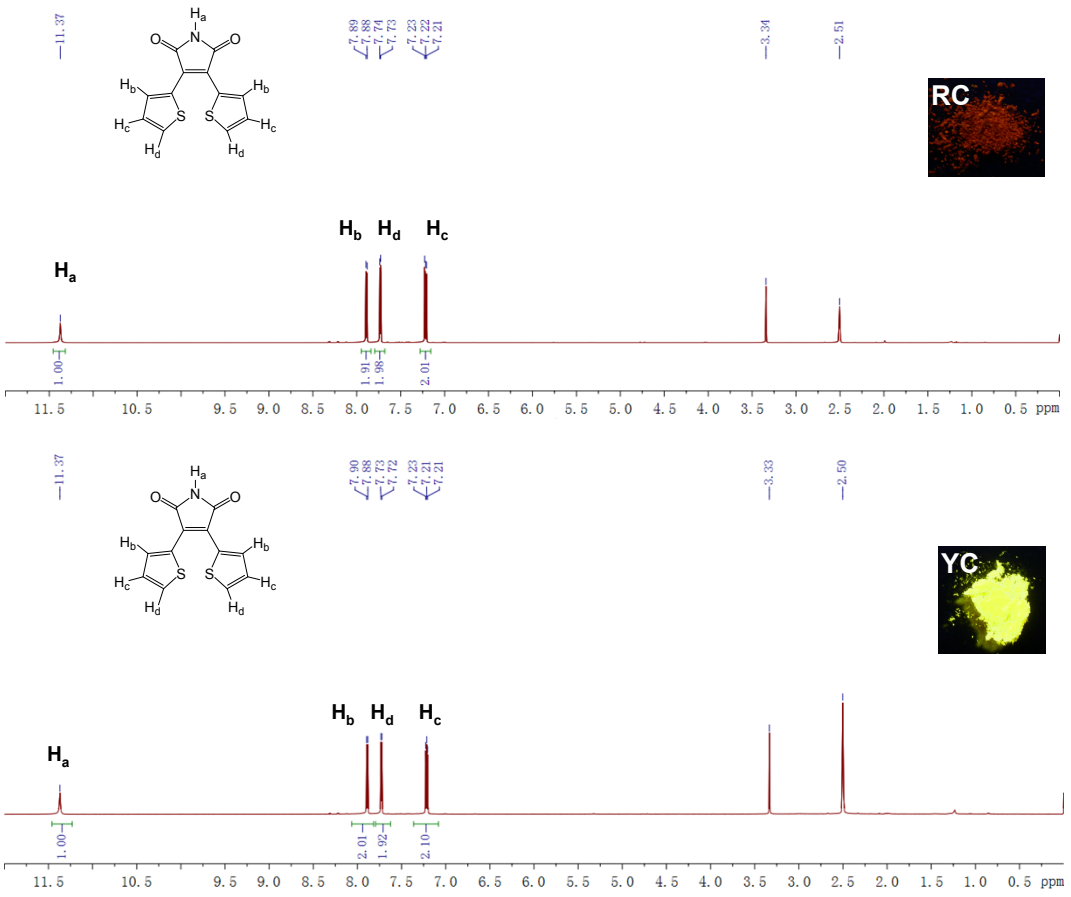

Fig. S2 [1]HNMR of RC and YC in d-DMSO.

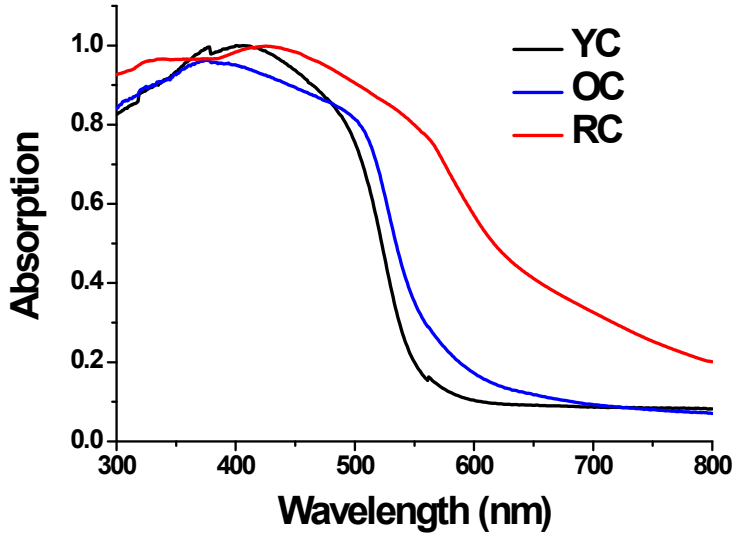

Fig. S3 The absorption spectra of YC, OC and RC.

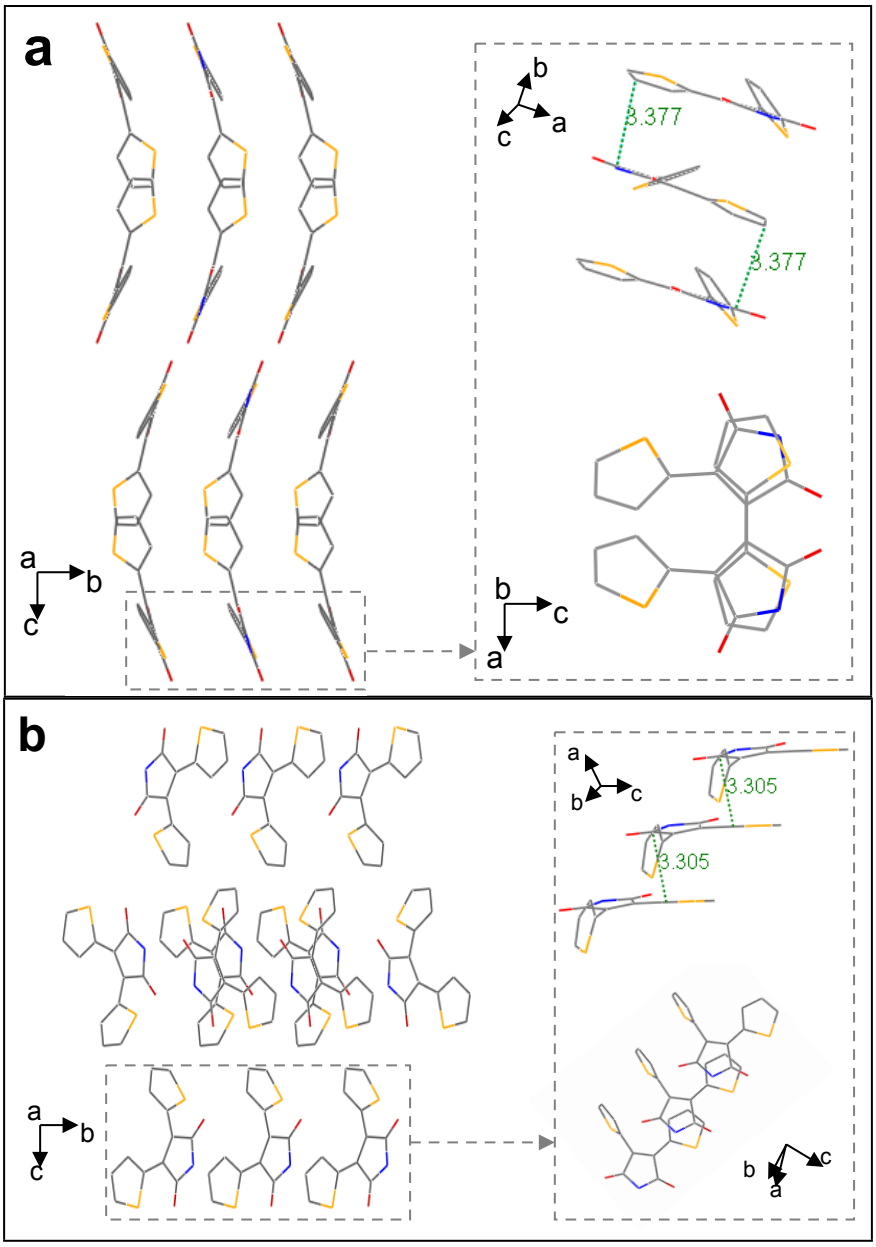

Fig. S4 The aggregation state of RC (a) and OC (b).

Table S3 Hydrogen bonds parameters for BTM crystal.

Crystals	D-H…A	d (D-H) (Å)	d (H…A) (Å)	d (D…A) (Å)	∠DHA (°)
RC	N1-H1…O2[a)]	0.84(2)	2.07(2)	2.905(4)	174(7)
	C6-H6…S1[b)]	0.93	2.82	3.739(4)	171.2
OC	N1-H1…O1[c)]	0.86	2.08	2.906(2)	162.1
	C6-H6…O1[d)]	0.93	2.51	3.367(3)	154.3

Symmetry codes: [a] 2-a, 1-b, 1-c; [b] 3/2-a, 1/2+b, c; [c] 1-a,1-b,1-c; [d] a, b-1, c.

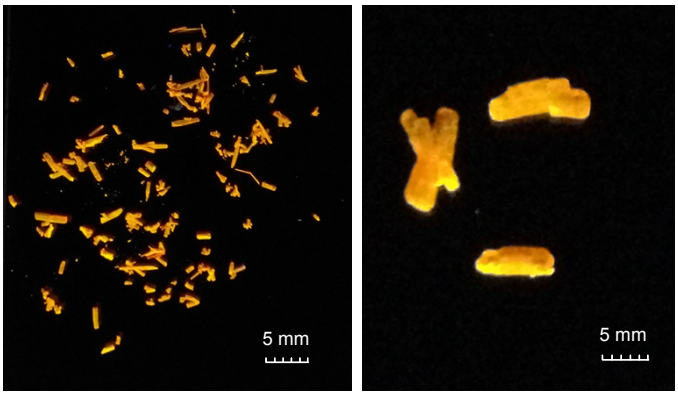

Fig. S5 Digital photo of OC crystals obtained quickly (left) and slowly (right) under UV lamp (365 nm).

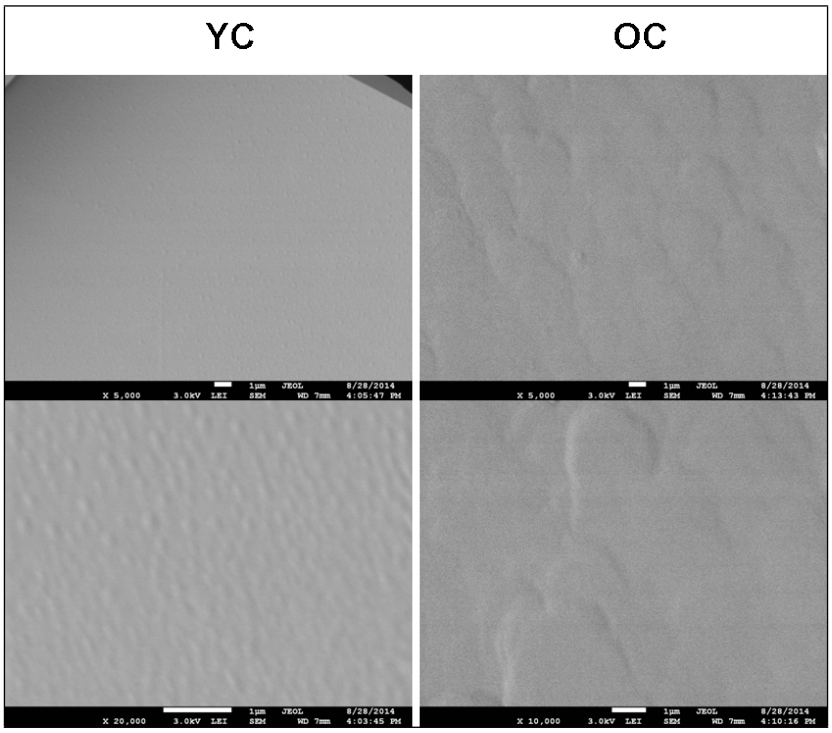

Fig. S6 SEM photo of YC and OC.

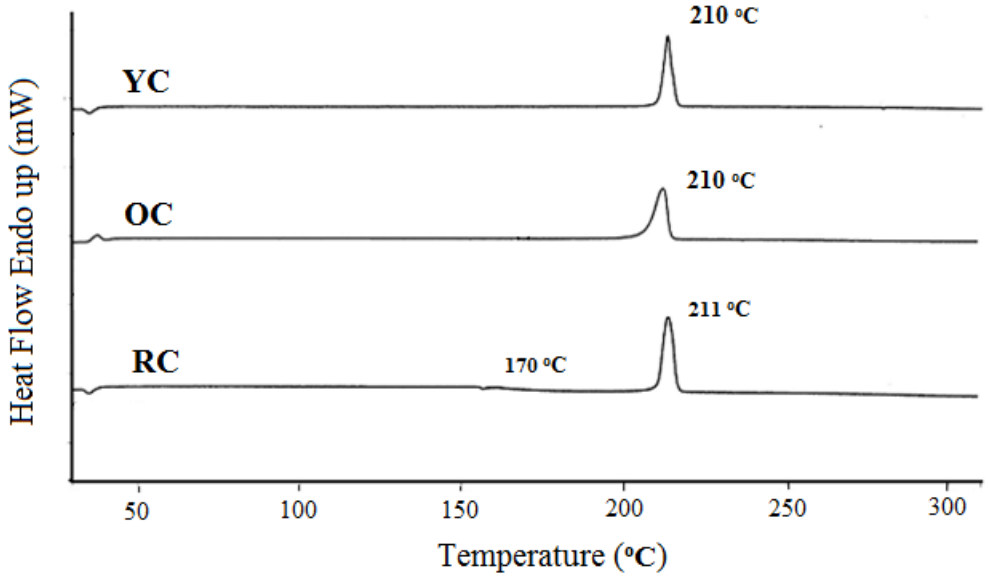

Fig. S7 DSC curves of RC, OC and YC.

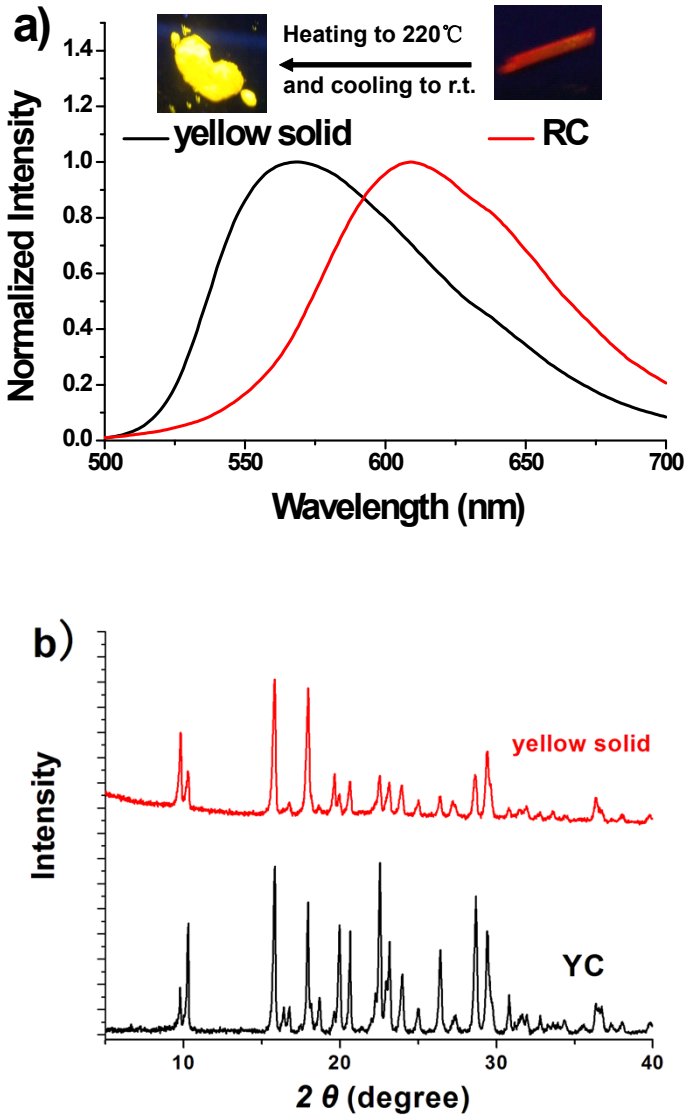

Fig. S8 Thermochromic Fluorescence of BTM crystals: a) Emission spectra of RC and yellow solid obtained from heat treatment of RC; b) Powder XRD patterns of the yellow solid and YC.

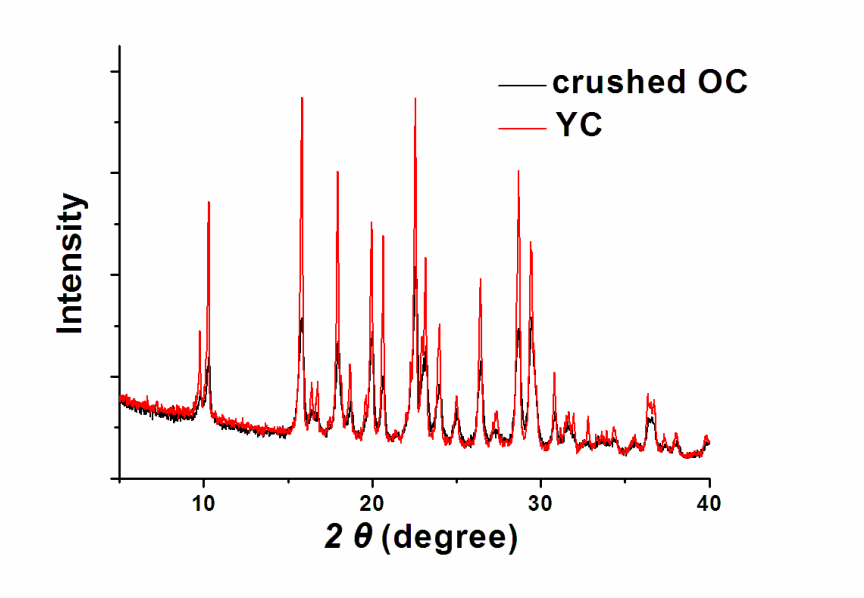

Fig. S9 Powder XRD patterns of the crushed OC solid and YC.

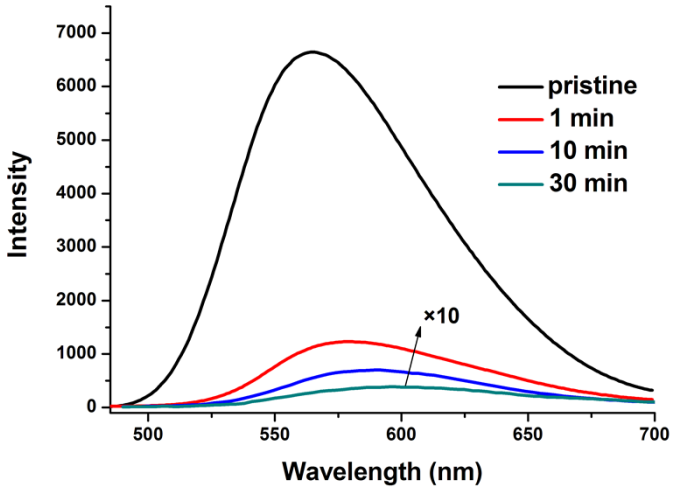

Fig S10 The effect of grinding time on the emission spectra of ground YC.

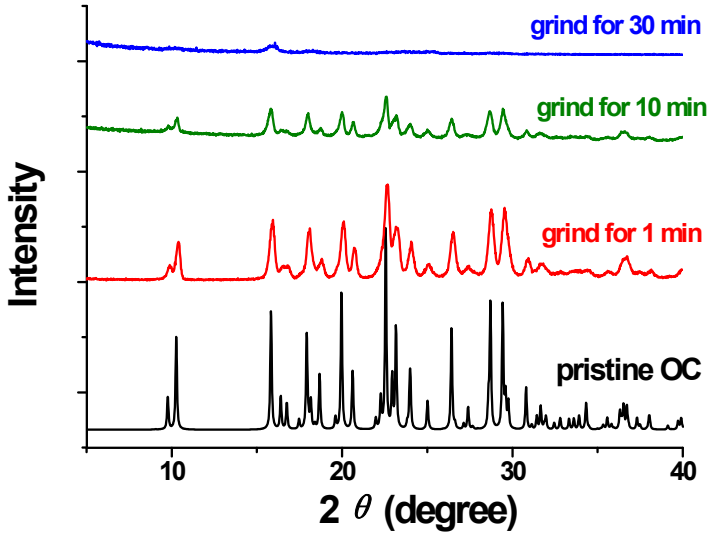

Fig S11 Powder XRD patterns of OC and ground OC. The pattern of OC ground for 30 min was obtained by using GIXRD.

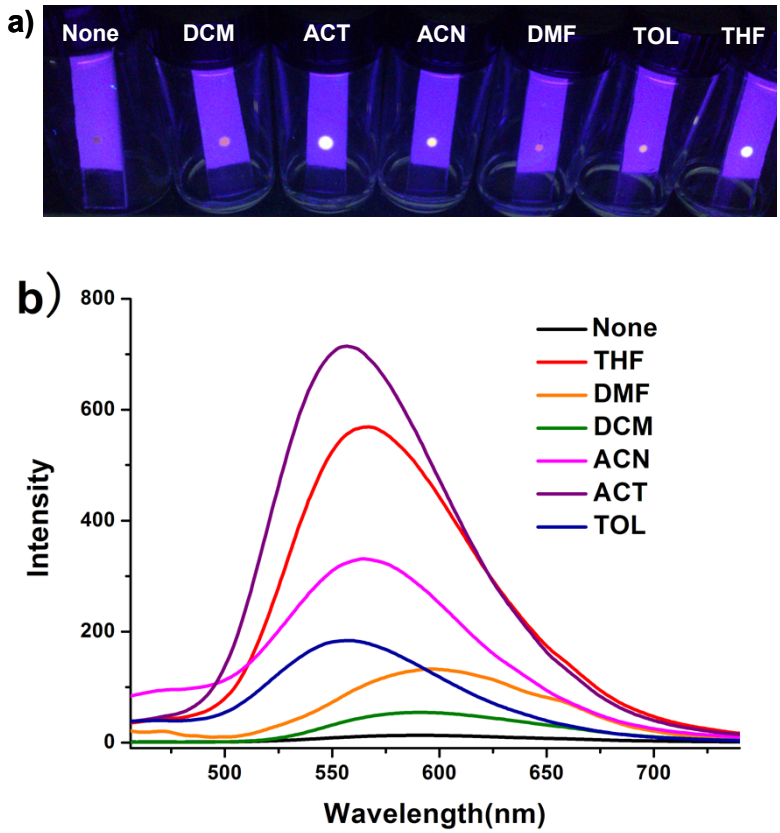

Fig. S12 a) Fluorescence of BTM solid in the silica gel plate was enhanced by various solvent vapors. b) The emission spectra of BTM solid in the silica gel plate under solvent vapors.

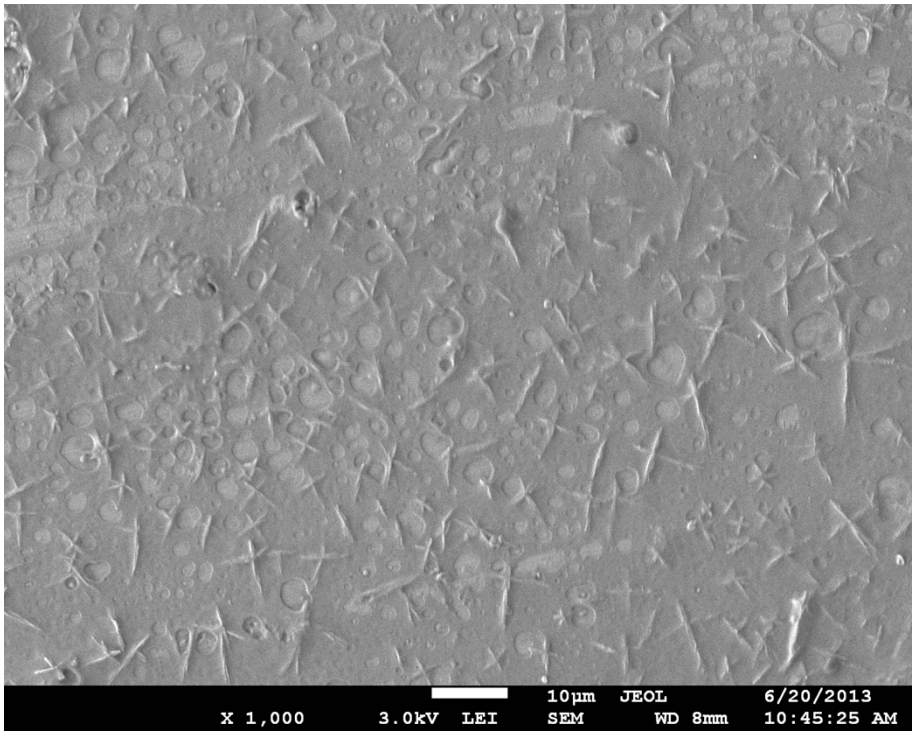

Fig. S13 The surface morphology of BTM (10 wt%) and PS composite film