

Reversible fluorescence switching and topochemical conversion in a organic AEE material: Polymorphism, deflection and nanofabrication mediated fluorescence tuning

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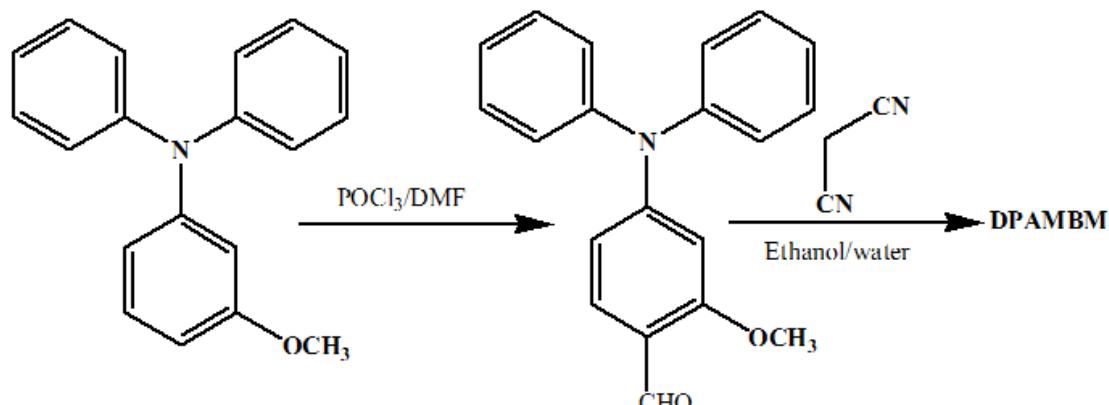
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Scheme S1. Synthesis of DPAMBM fluorophore.

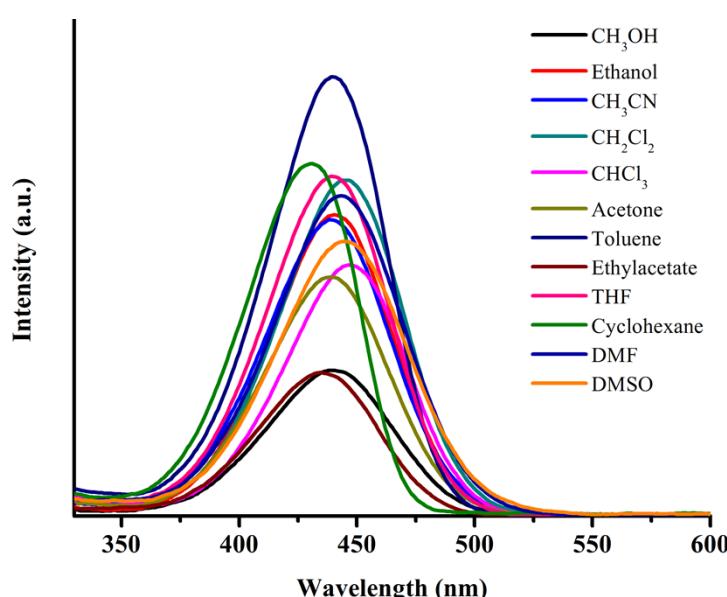


Figure S1. Absorption spectra of DPAMBM in different solvents.

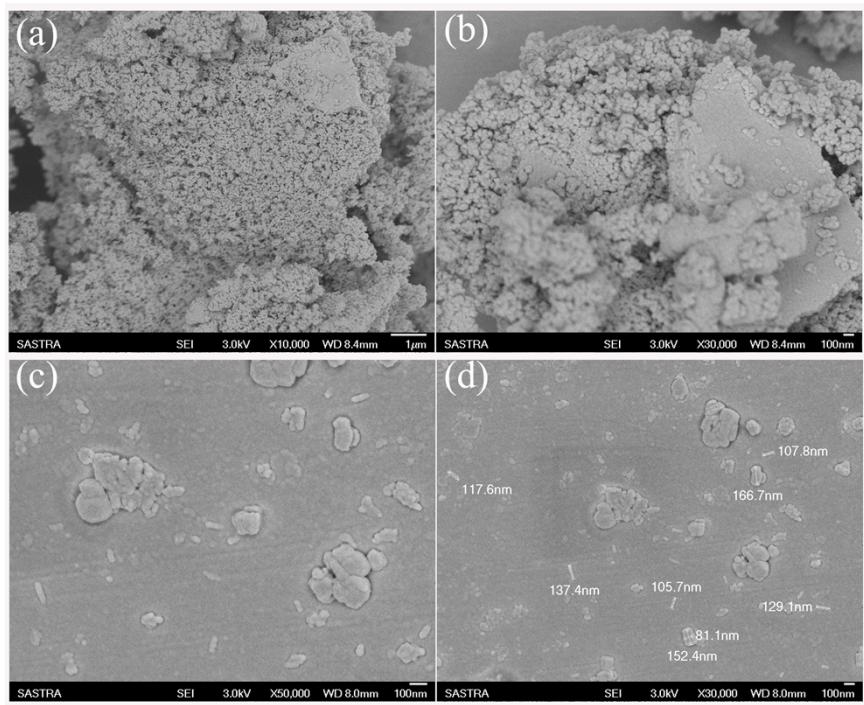


Fig. S2. FE-SEM images of DPAMBM-CH₃CN injected into water (100 %), (a,b) initial and (c,d) after 24 h.

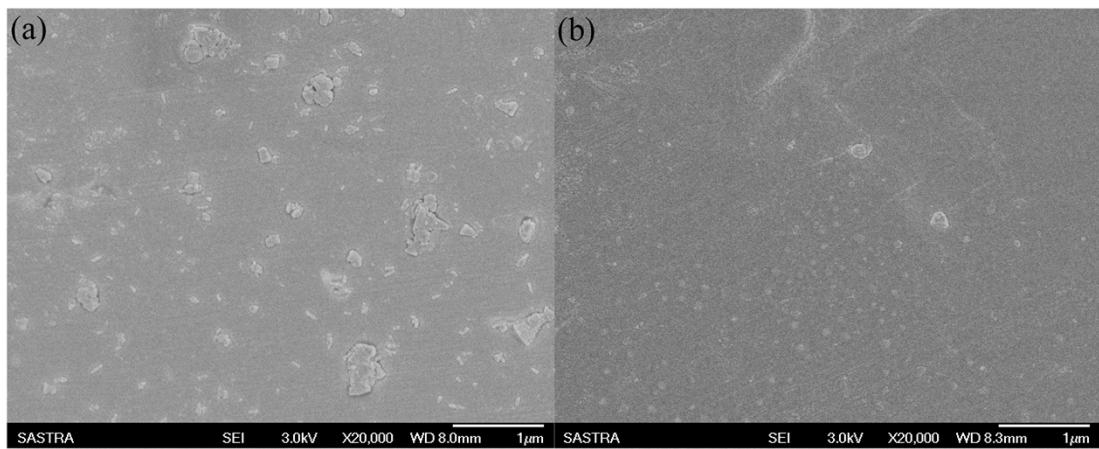


Fig. S3. FE-SEM images of DPAMBM injected in to water after 24 h(a) 100 % and (b) 90 %.

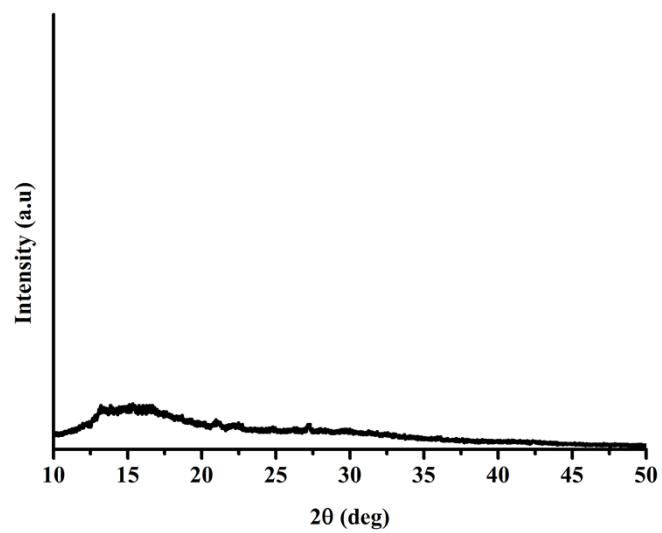


Fig. S4. PXRD pattern of DPAMBM nanoparticles fabricated in water (100 %).

Table S1. Crystal data and structure refinement for DPAMBM-1 (**CCDC No. 1039161**).

Identification code	CCDC No. 1039161	
Empirical formula	C ₂₃ H ₁₇ N ₃ O	
Formula weight	351.39	
Temperature	100(2) K	
Wavelength	0.60999 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 16.858(3) Å	α = 90°.
	b = 12.594(3) Å	β = 98.44(3)°.
	c = 17.493(4) Å	γ = 90°.
Volume	3673.7(13) Å ³	
Z	8	
Density (calculated)	1.271 Mg/m ³	
Absorption coefficient	0.059 mm ⁻¹	
F(000)	1472	
Crystal size	0.300 x 0.200 x 0.200 mm ³	
Theta range for data collection	1.739 to 24.999°.	
Index ranges	-23<=h<=23, -17<=k<=17, -24<=l<=24	
Reflections collected	18323	
Independent reflections	5069 [R(int) = 0.0201]	
Completeness to theta = 21.469°	98.1 %	
Absorption correction	Empirical	
Max. and min. transmission	0.988 and 0.983	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5069 / 0 / 245	
Goodness-of-fit on F ²	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0389, wR2 = 0.1088	
R indices (all data)	R1 = 0.0408, wR2 = 0.1106	
Largest diff. peak and hole	0.403 and -0.223 e.Å ⁻³	

Table S2.Crystal data and structure refinement for DPAMBM-2 (**CCDC No. 1039160**).

Identification code	CCDC No. 1039160		
Empirical formula	C ₂₃ H ₁₇ N ₃ O		
Formula weight	351.39		
Temperature	100(2) K		
Wavelength	0.60999 Å		
Crystal system	Monoclinic		
Space group	C2/c		
Unit cell dimensions	a = 34.743(7) Å	α = 90°.	
	b = 6.9070(14) Å	β = 110.18(3)°.	
	c = 16.066(3) Å	γ = 90°.	
Volume	3618.7(14) Å ³		
Z	8		
Density (calculated)	1.290 Mg/m ³		
Absorption coefficient	0.060 mm ⁻¹		
F(000)	1472		
Crystal size	0.500 x 0.150 x 0.150 mm ³		
Theta range for data collection	2.587 to 24.999°.		
Index ranges	-48≤h≤48, -9≤k≤9, -22≤l≤22		
Reflections collected	17907		
Independent reflections	5001 [R(int) = 0.0237]		
Completeness to theta = 21.469°	98.6 %		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	5001 / 0 / 245		
Goodness-of-fit on F ²	1.035		
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.1068		
R indices (all data)	R1 = 0.0405, wR2 = 0.1085		
Largest diff. peak and hole	0.470 and -0.267 e.Å ⁻³		

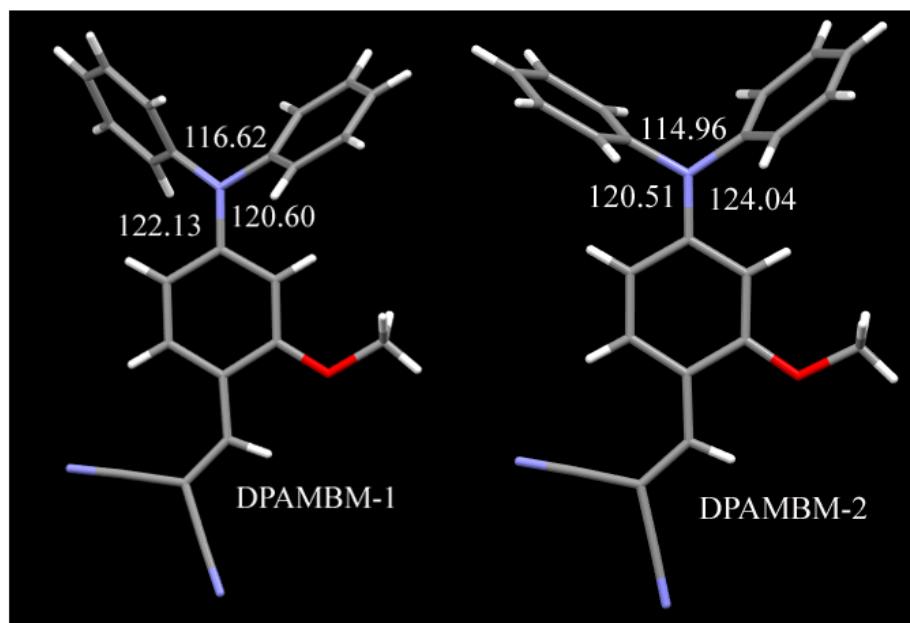


Fig. S5. Molecular conformation of DPAMBM in DPAMBM-1 and DPAMBM-2. Angles are given in the figure.

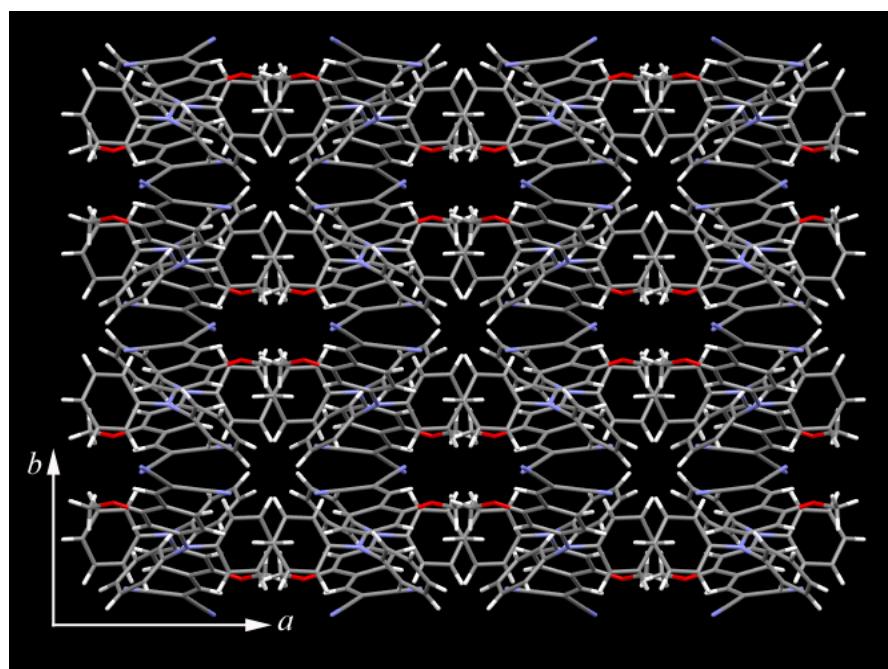


Fig. S6. Molecular packing of DPAMBM-1 in the crystal lattice along *ab*-plane.

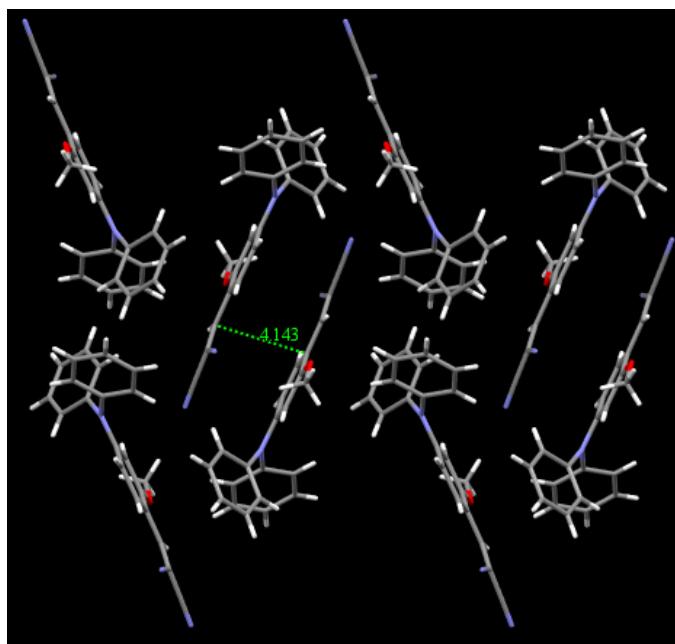


Fig. S7. Molecular packing of DPAMBM-1. The doted line shows the distance between two DPAMBM molecule in the crystal lattice.

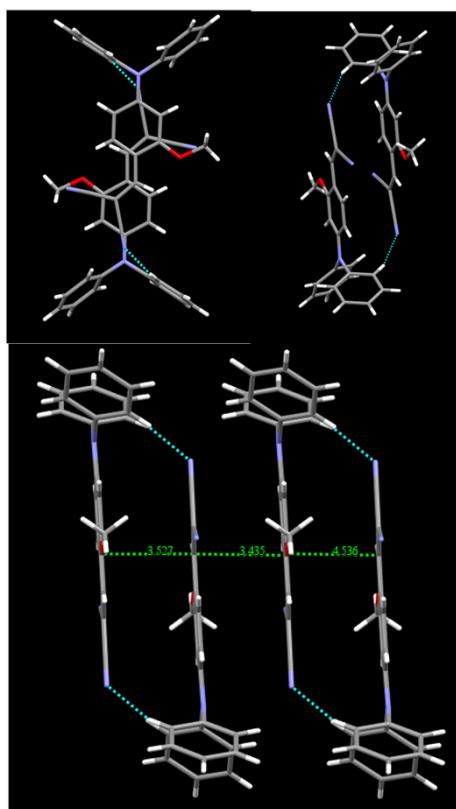


Fig. S8. Dimer formation of DPAMBM via H-bonding in the crystal lattice of DPAMBM-1 and π - π interactions between the dimers.

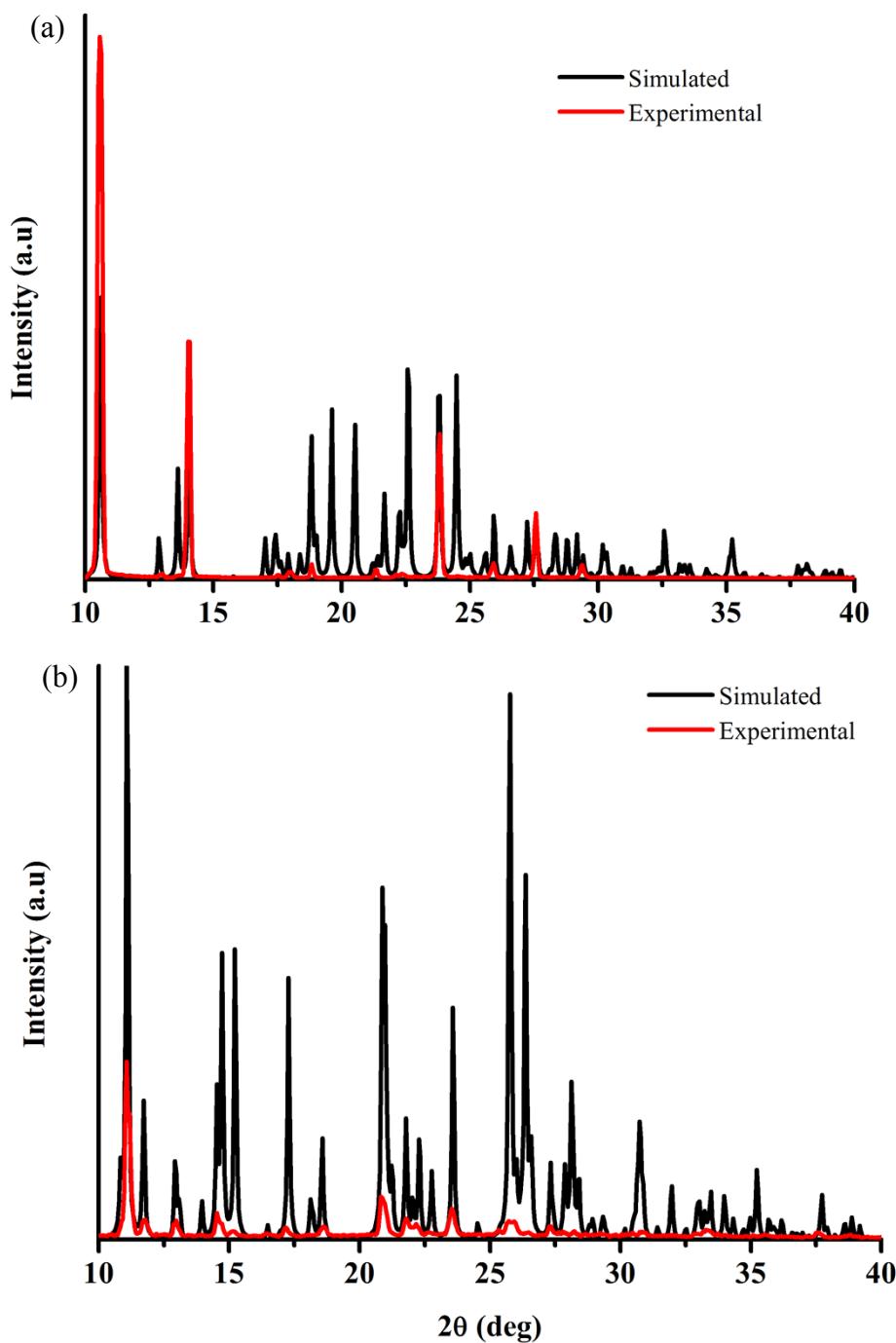


Fig. S9. PXRD pattern of experimental and stimulated patter of (a) DPAMBM-1 and (b) DPAMBM-2.

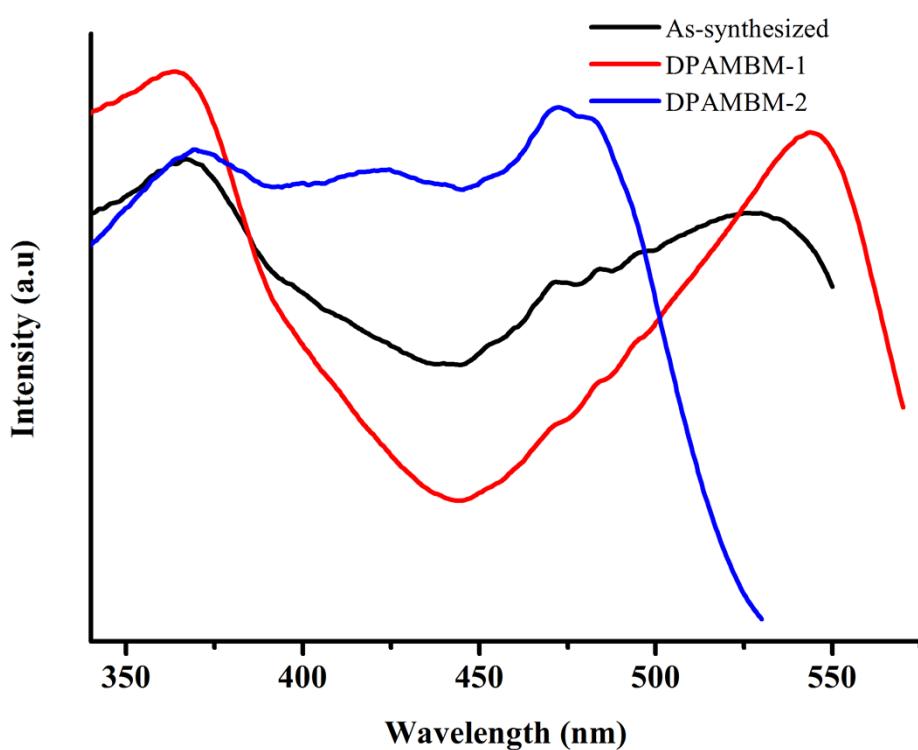


Fig. S10. Excitation spectra of as-synthesized DPAMBM powder, DPAMBM-1 and DPAMBM-2.

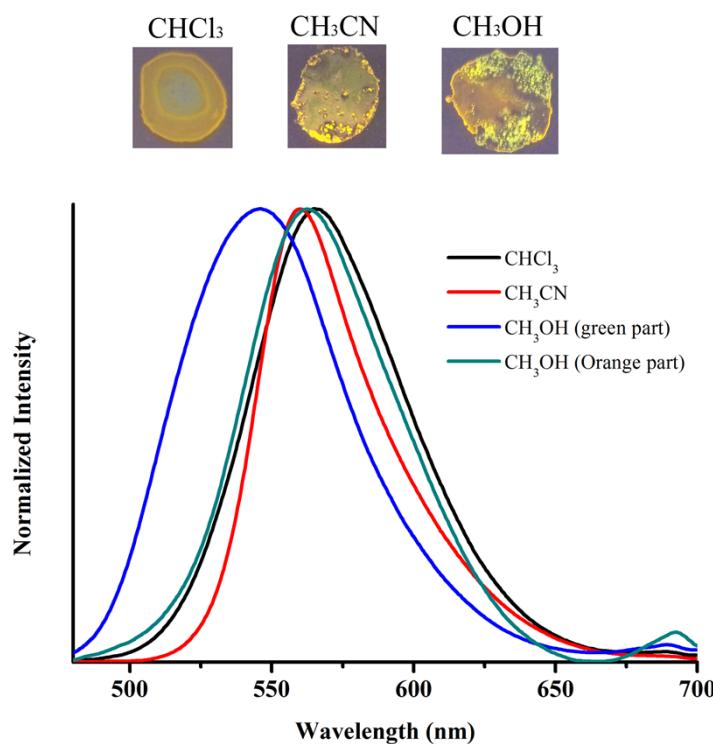


Fig. S11. Digital images and fluorescence spectra of thin film fabricated by drop-casting approach from different solvents.

Table S3. Cell indexing data of DPAMBM single crystals grown from different solvents.

	DPAMBM-1	EtOAc	IPA	THF-1	DPAMBM-2	THF-2
<i>a</i> (Å)	16.858(3)	16.861(3)	16.886(3)		34.743(7)	34.739(7)
<i>b</i> (Å)	12.594(3)	12.600(3)	12.641(3)		6.9070(14)	6.9080(14)
<i>c</i> (Å)	17.493(4)	17.497(4)	17.519(4)		16.066(3)	16.065(3)
α (°)	90	90	90		90	90
β (°)	98.44(3)	98.43(3)	98.36(3)		110.18(3)	110.20(3)
γ (°)	90	90	90		90	90

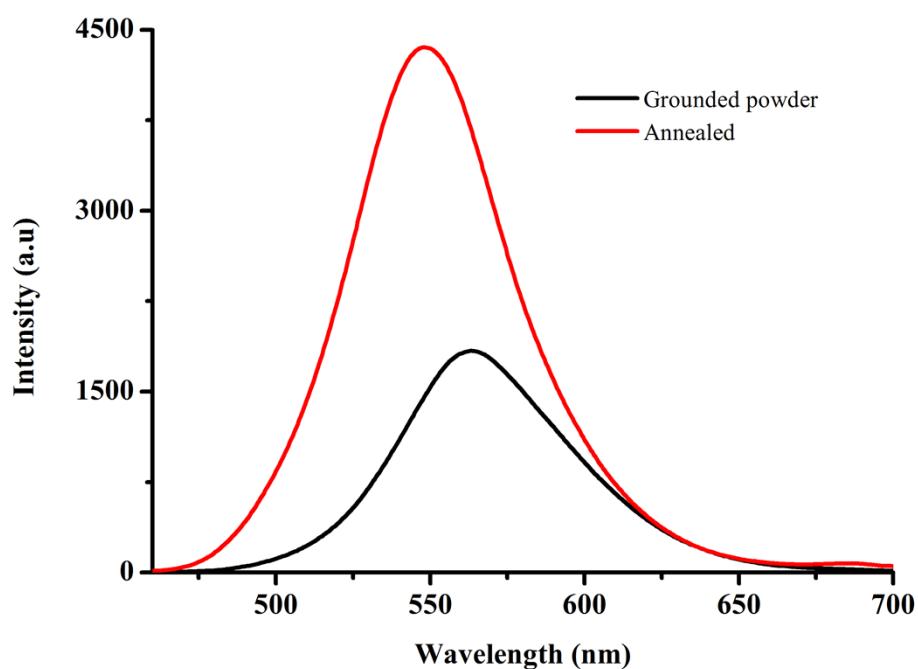


Fig. S12. Fluorescence spectra of DPAMBM-1 strongly grounded powder and annealed at 120 °C.

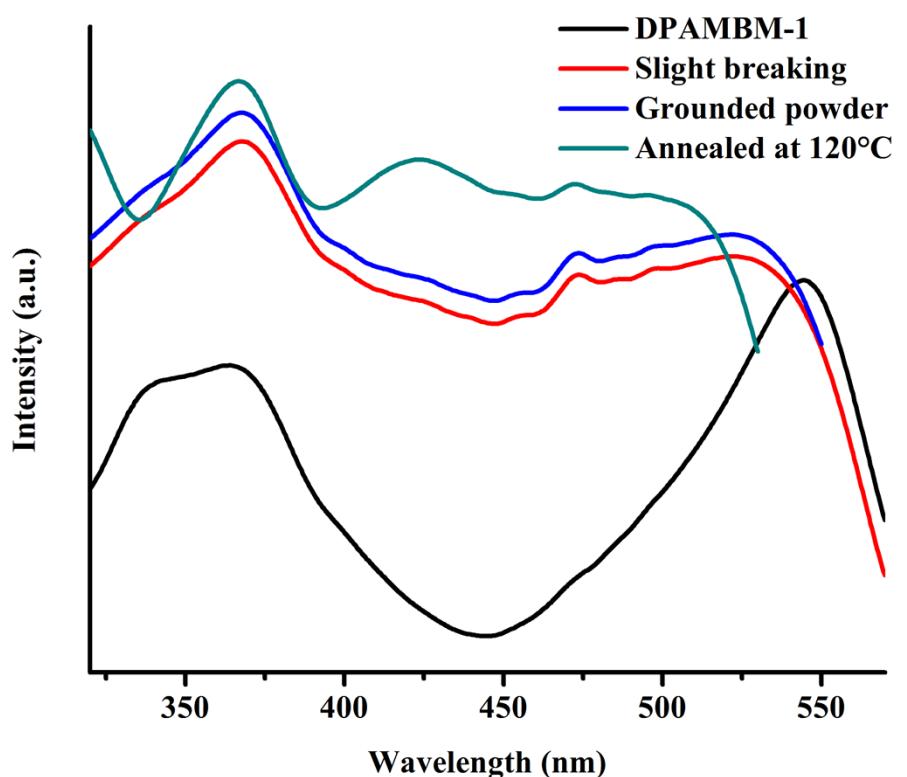


Fig.

S13. Excitation spectra of as-synthesized DPAMBM-1, slightly broken, strongly grounded powder and annealed form.

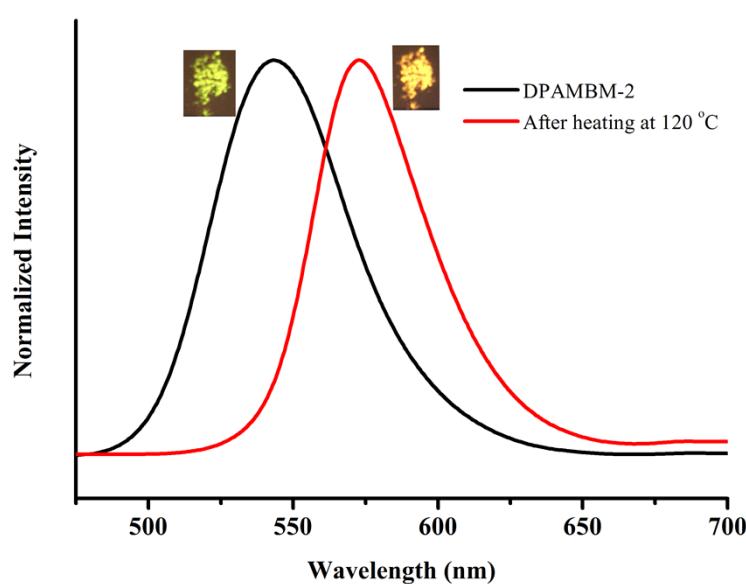


Fig. S14. Fluorescence spectra of DPAMBM-2 crystals before and after heating.

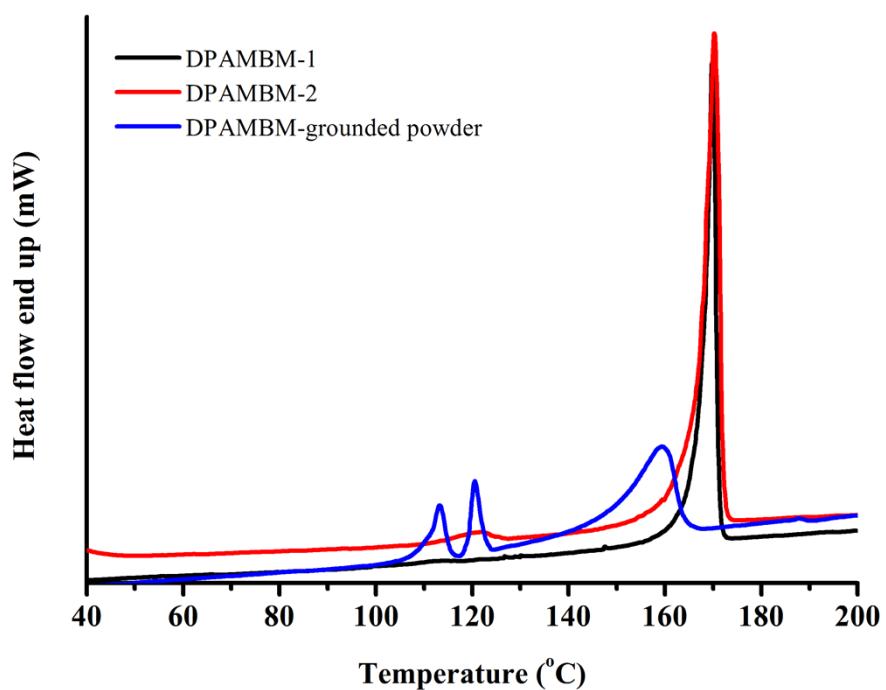


Fig. S15. DSC spectra of DPAMBM.