Supporting Information (SI)

Light/Temperature- Enhanced Emission Characterstic of Malononitrile-Containing Hexaphenyl-1,3-Butadiene Derivatives: the Hotter, the Brighter

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1.1 Instrumentations and Methods

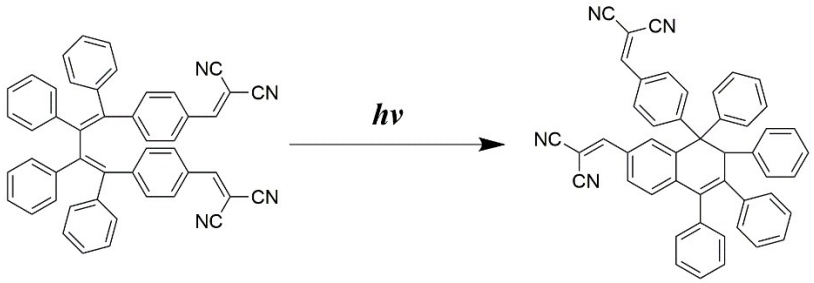
The UV-vis spectra were recorded on a TU-1901 UV-Vis spectrophotometer (Beijing Purkinje General Instrument Co., Ltd.). Photoluminescence (PL) spectra were collected on a Hitachi F-7000 fluorescence spectrophotometer at room temperature. X-ray crystal structure analyses were measured on Bruker-AXS SMART APEX2 CCD diffractometer. Powder X-ray diffraction (PXRD) was performed using monochromatized Cu-Ka (l ¼ 1.54,178 Å) incident radiation with a Shimadzu XRD-6000 instrument operating at 40 kV voltage and 50 mA current.

The synthetic routes and characterization of HPB-CN was given and analyzed in previous research[S1]. Characterization of HPB-CN include 1H-NMR spectra, 13C-NMR spectra, MS data and IR were not repeat here.

1.2 Crystal data

Crystal data for HPB-CN: C_{48} H_{30} N_4; Formula weight: 662.76; monoclinic; P21/c; a=14.768(16), b=15.377(17), c=16.689(18) Å; α/°=90.00°, β/°=90°, γ/°=90.0; V=3790(7) $Å^3$; Z=4; ρ_{calc} =1.162 Mg/m^3; μ=0.069 mm^{-1}; F(000)= 1384; T= 100.7 K; 2θ= 1.801 to 25.906°; 3638 independent reflections (Rint=0.1052); GOF on F_2= 0.943; R_1 = 0.1352, wR_2 = 0.1904 (all data); Δe 0.201 and -0.196 e.$Å^{-3}$

CCDC 1535584 of HPB-CN contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Scheme S1. Photocyclization route of HPB-CN.

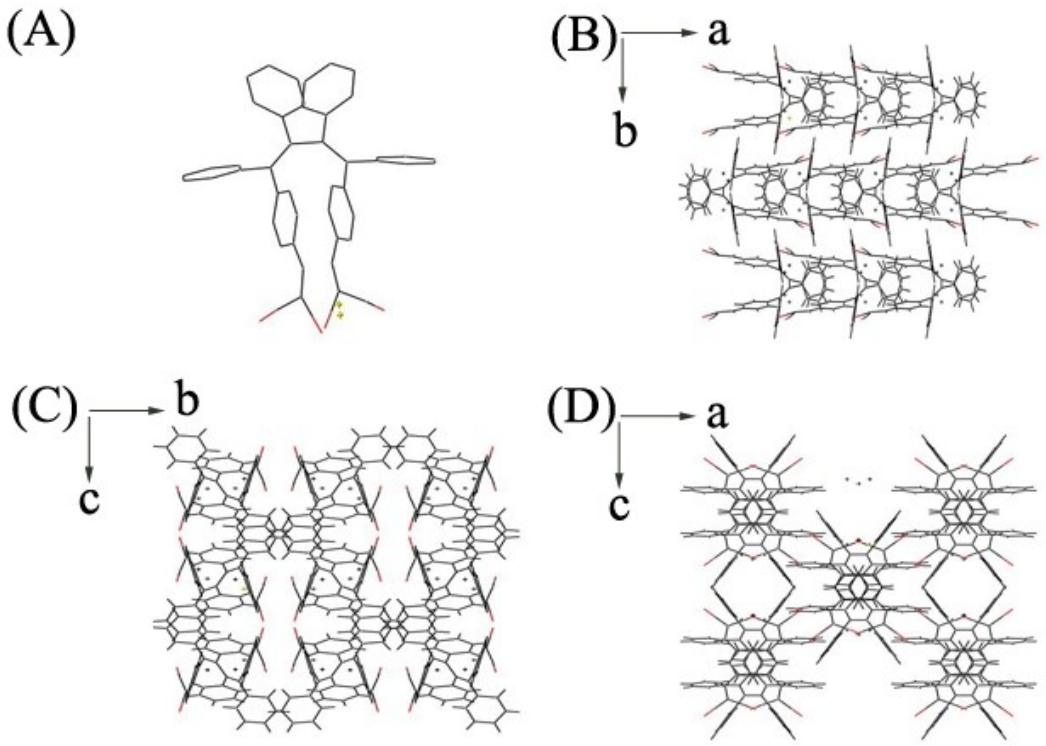
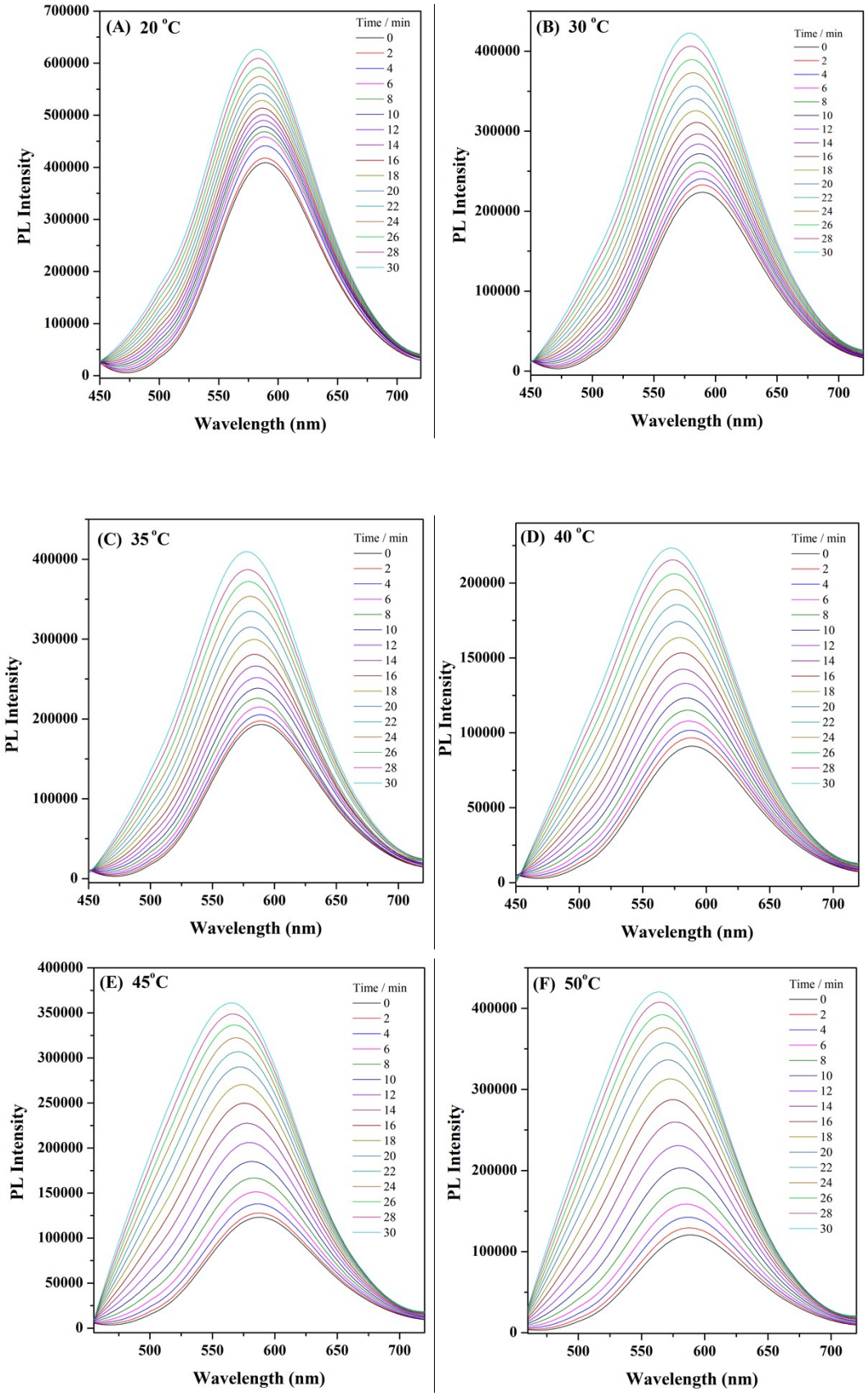


Figure S1 Molecular packing patterns of HPB-CN in the crystalline state, determined by single-crystal X-ray crystallography

Figure S2. Pictures of filter paper strips before and after treatments (Heating at 90 ^{o}C for 20 min).


(A) 20 °C
(B) 30 °C
(C) 35 °C
(D) 40 °C
(E) 45°C
(F) 50°C
Time / min
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
PL Intensity
Wavelength (nm)

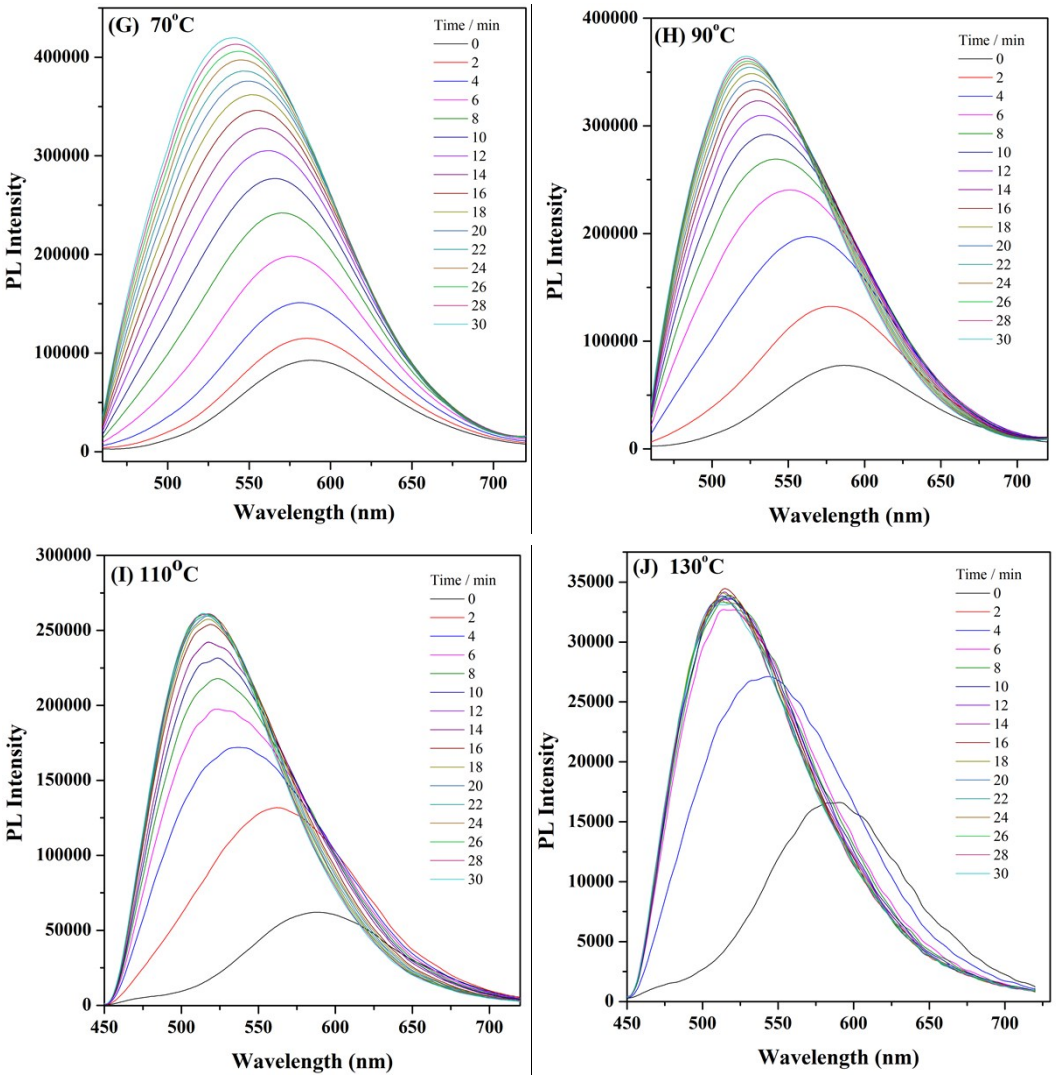


Figure S3. PL spectra of filter paper strips at 20, 30, 35, 40, 45, 50, 70, 90, 110 and 130 °C for 30 min.

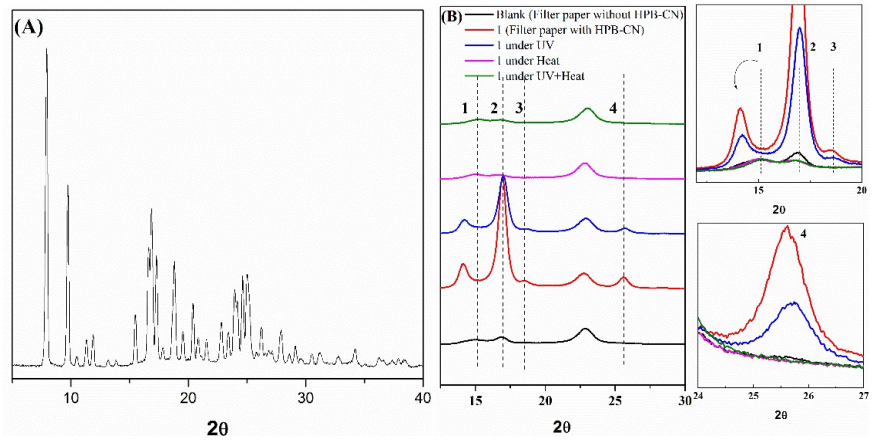


Figure S4 XRD patterns of HPB-CN powder and filter paper strips.

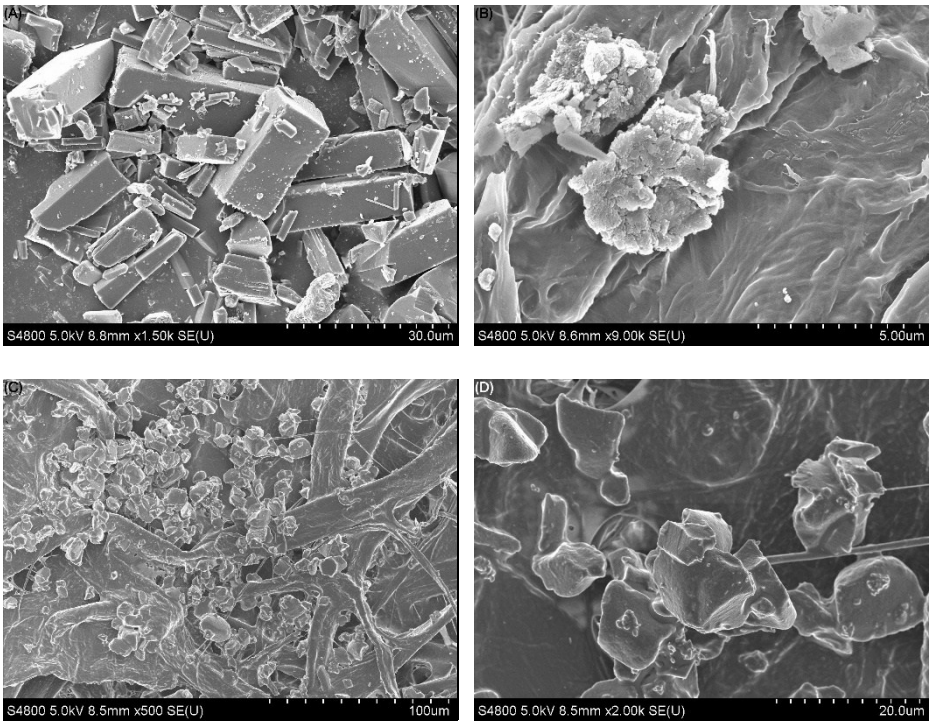


Figure S5 SEM of original HPB-CN powder (A), dropped on filter paper strips before (B) and after (C), (D) treatment (UV and Heating at 90 °C for 20 min)

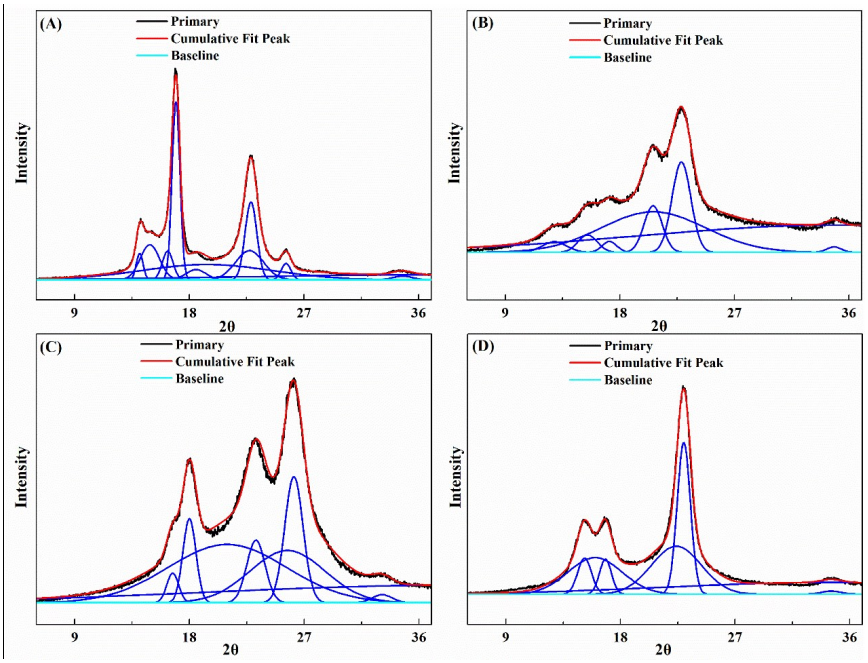


Figure S6 XRD patterns of HPB-CN dropped on (A) filter paper strip; (B) cotton-linen cloth; (C) polyester fabrics; (D) filter paper strip after quenching.[S2]

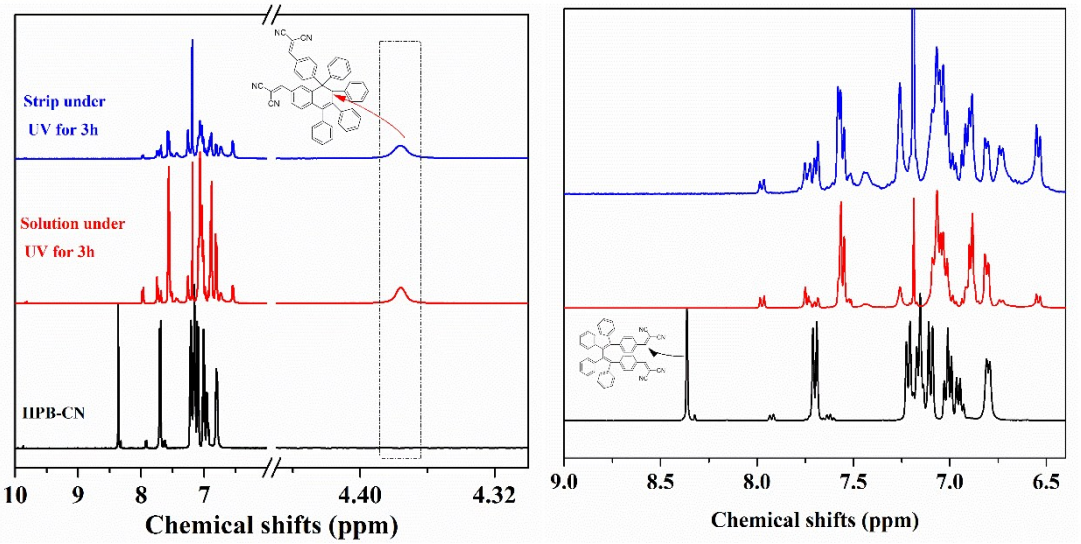


Figure S7 ^{1}H-NMR spectra of powder, solution and filter paper strips of HPB-CN under UV light for 3 hours.

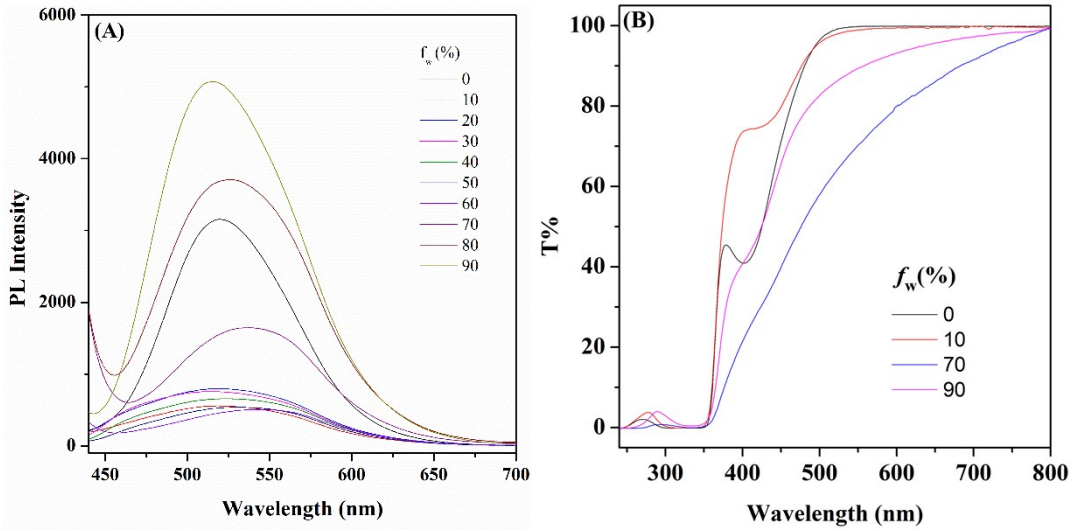


Figure S8 (A) PL spectra of HPB-CN in mixture of water and THF after UV light for 3 hours; (B) T% spectra of HPB-CN in mixture of water and THF after UV light for 3 hours. [HPB-CN] = 1×10^{-4} M, λ_{ex} = 410 nm

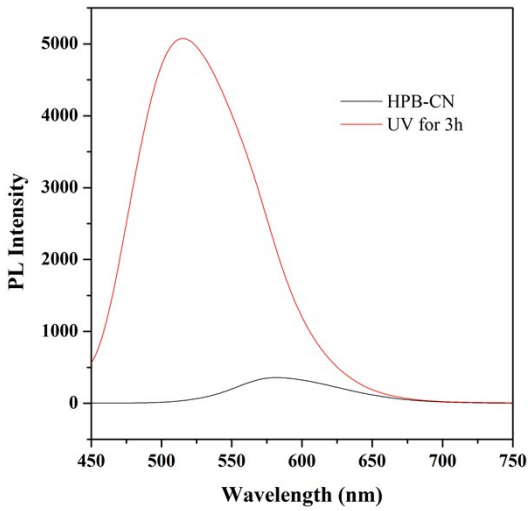
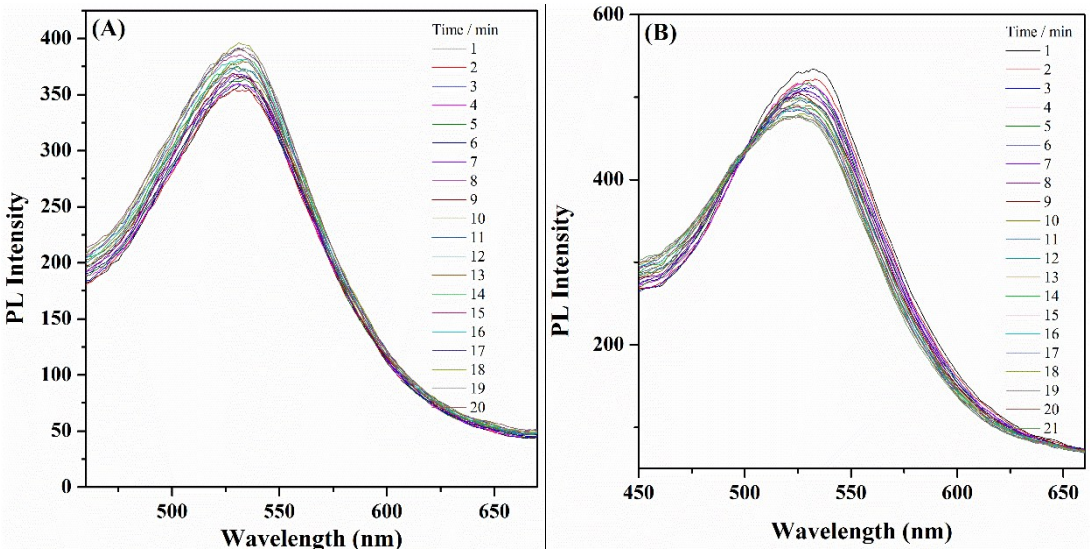


Figure S9 PL spectra of HPB-CN in mixture of water and THF before and after UV light for 3 hours



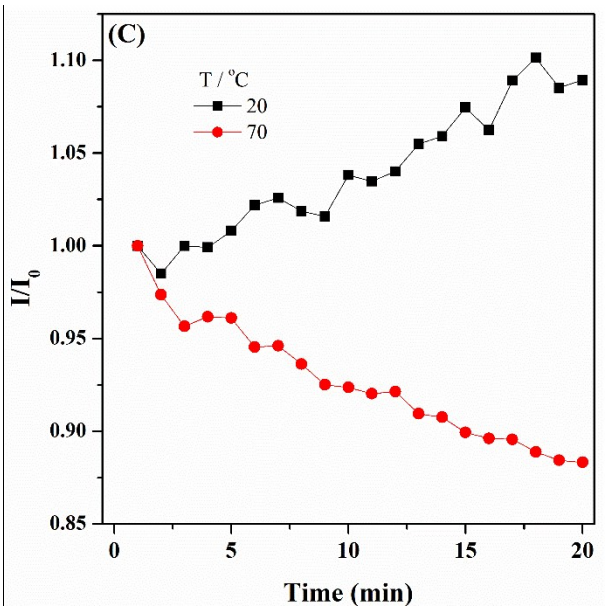


Figure S10 PL spectra of photocyclization filter paper strips at (A) 20 °C (B) 70 °C and (C) Correlation between the net change in PL intensity I/I_0 for 30 min.

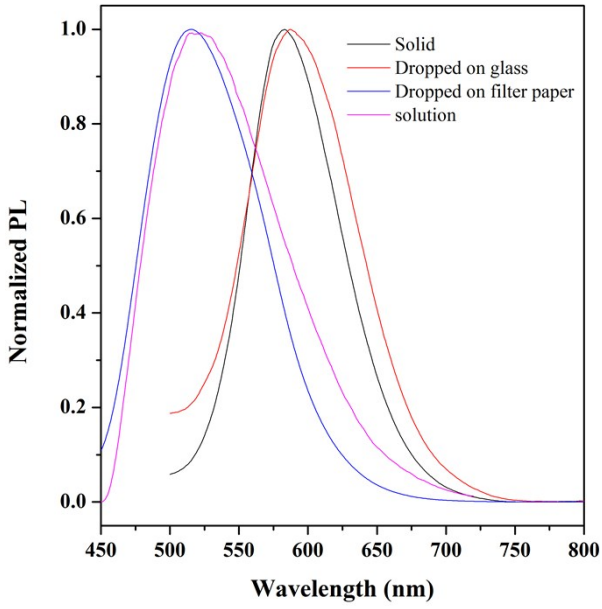


Figure S11 PL spectra of HPB-CN after UV light for 20 min.

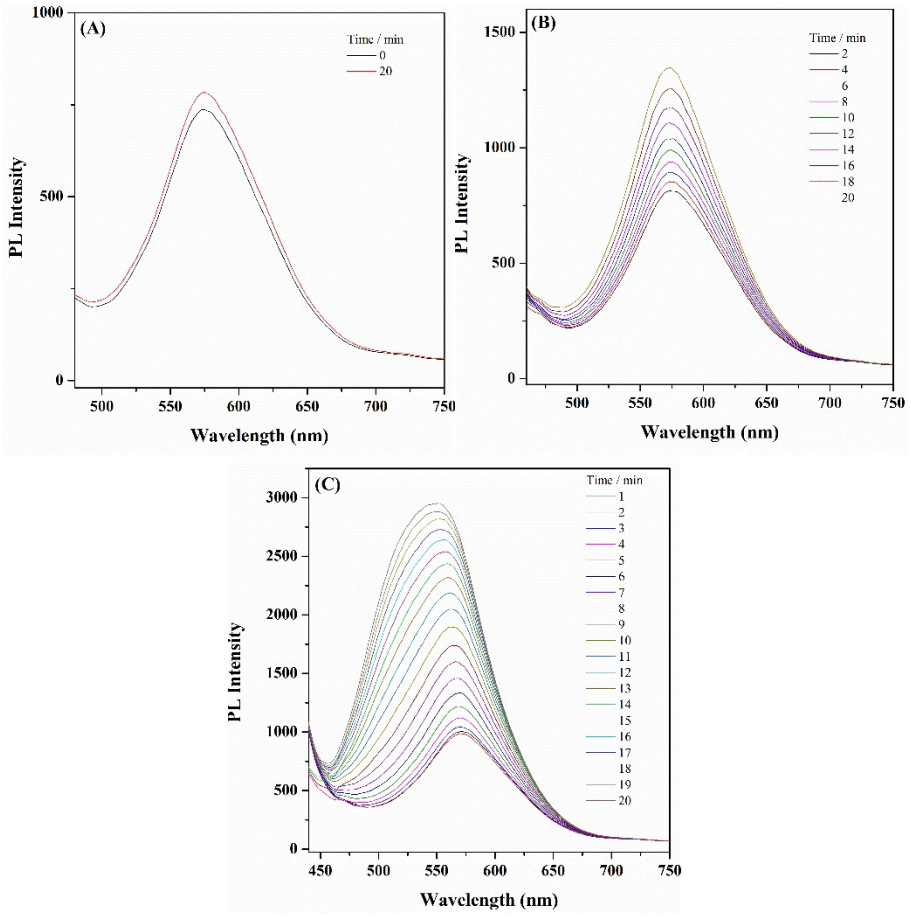


Figure S12 Fluorescence intensity of filter paper strips exposed to UV light with interval exposed time (A) per 20 min (B) per 2 min (C) per 1 min

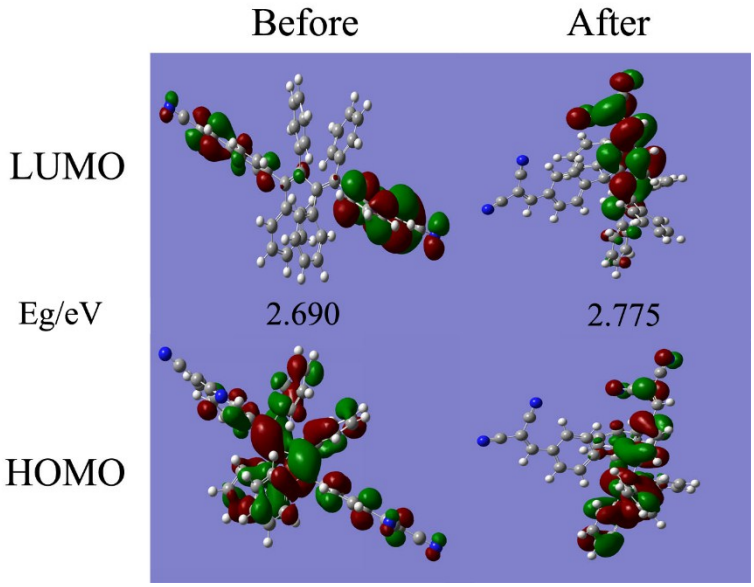


Figure S13. B3LYP/6-31G (d) calculated molecular orbital amplitude plots of HOMO and LUMO level of HPB-CN before and after photocyclization.

1 L. W. Kong, Y. H. Zhang, H. L. Mao, X. L. Pan, Y. Tian, Z. L. Tian, X. K. Zeng, J. B. Shi, B. Tong and Y. P. Dong, *Faraday Discuss.,* 2017, **196**, 101-111.
2 A. L. Rubio, B. M. Flanagan, E. P. Gilbert and M. J. Gidley, *Biopolymers*, 2008, **89**, 761-767.