Supporting Information

Fast Photo Stimulus Responsive Ultralong Room-temperature Phosphorescence Behavior of Benzoic Acid Derivatives @Boric acid

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I. Physical and chemical properties of BADs@BA

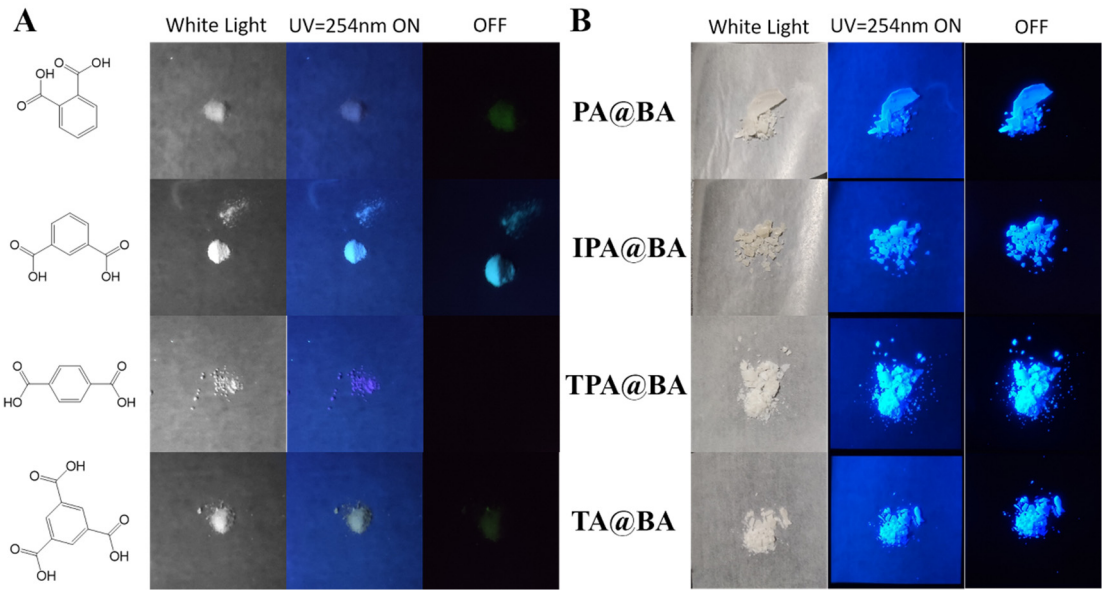


Figure S1. A) The fluorescence and phosphorescence images of phthalic acid (PA), isophthalic acid (IPA), terephthalic acid (TPA), and trimesic acid (TA) under 254 nm light. B) The fluorescence and phosphorescence images of BADs@BA.

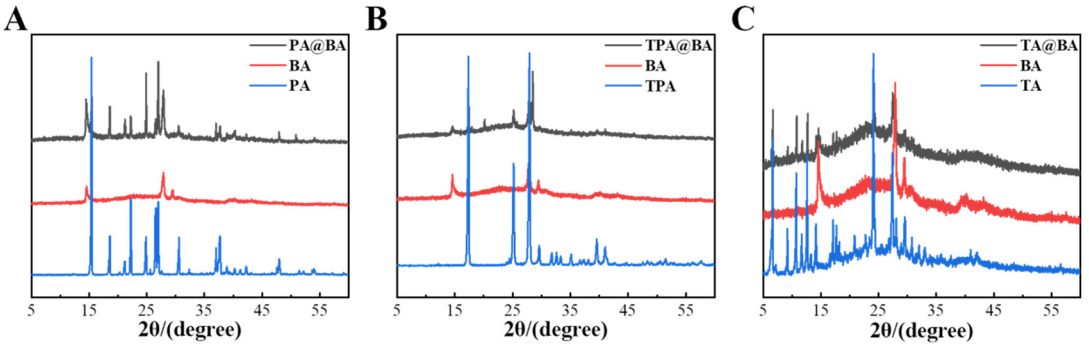


Figure S2. B) PXRD patterns of BA, PA, and PA@BA, respectively. B) PXRD patterns of BA, TPA, and TPA@BA. C) PXRD patterns of BA, TA, and TA@BA, respectively.

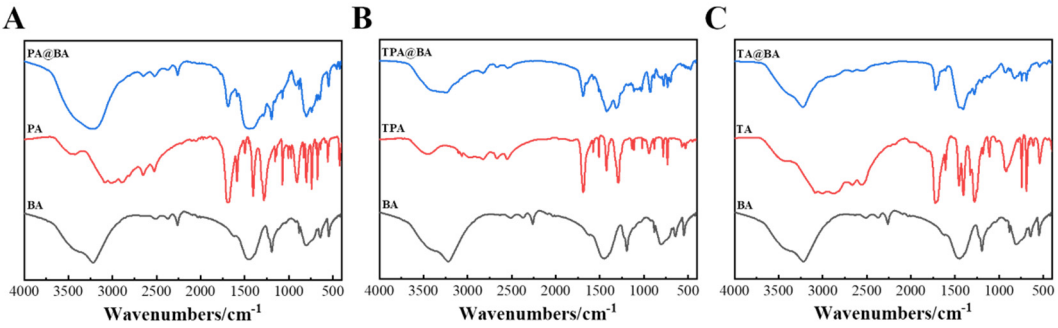


Figure S3. A) FT-IR spectra of BA, PA, and PA@BA, respectively. B) FT-IR spectra of BA, TPA, and TPA@BA, respectively. C) FT-IR spectra of BA, TA, and TA@BA, respectively.

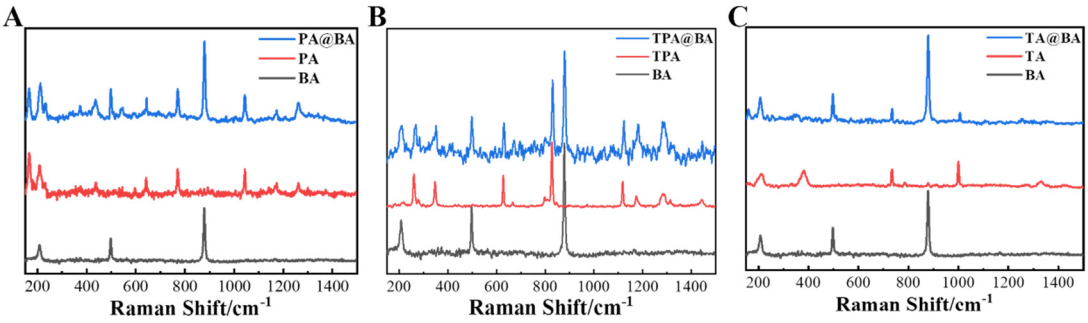


Figure S4. A) Raman spectra of BA, PA, and PA@BA, respectively. B) Raman spectra of BA, TPA, and TPA@BA, respectively. C) Raman spectra of BA, TA, and TA@BA, respectively.

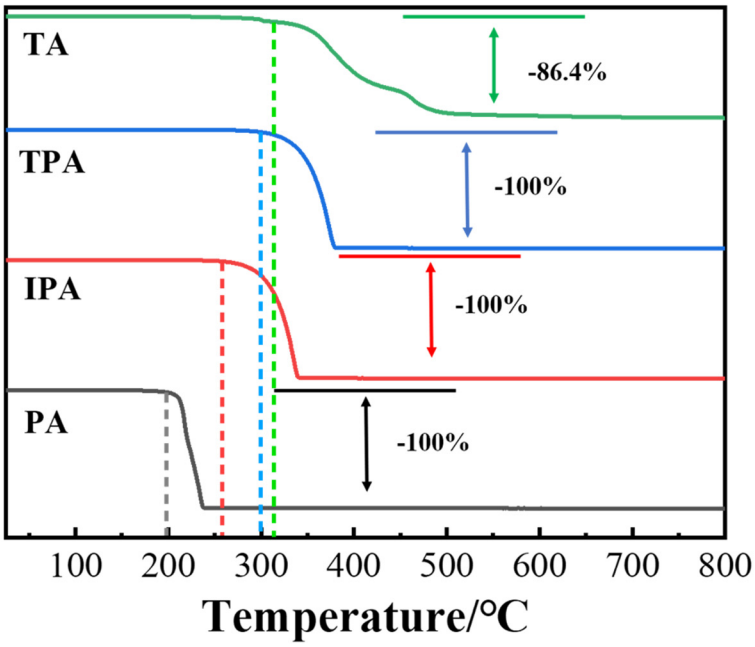
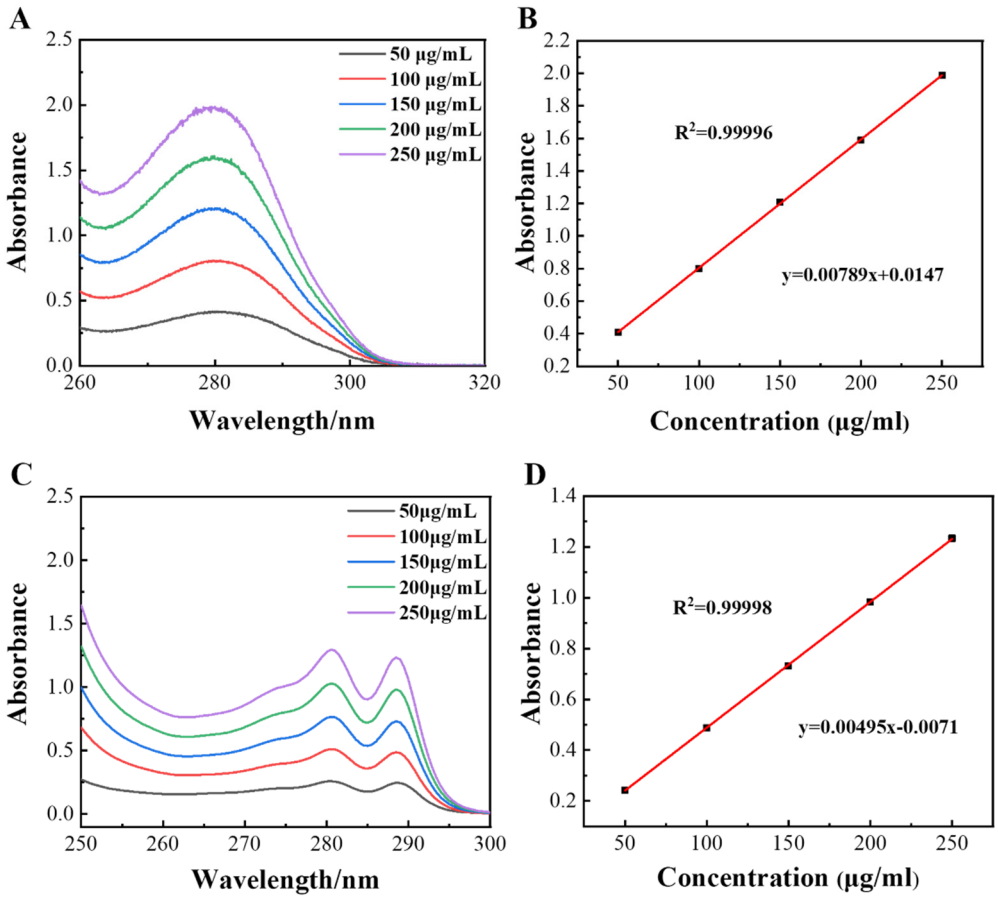


Figure S5. Thermogravimetric analysis curves of phthalic acid (PA), isophthalic acid (IPA), terephthalic acid (TPA), and trimesic acid (TA).



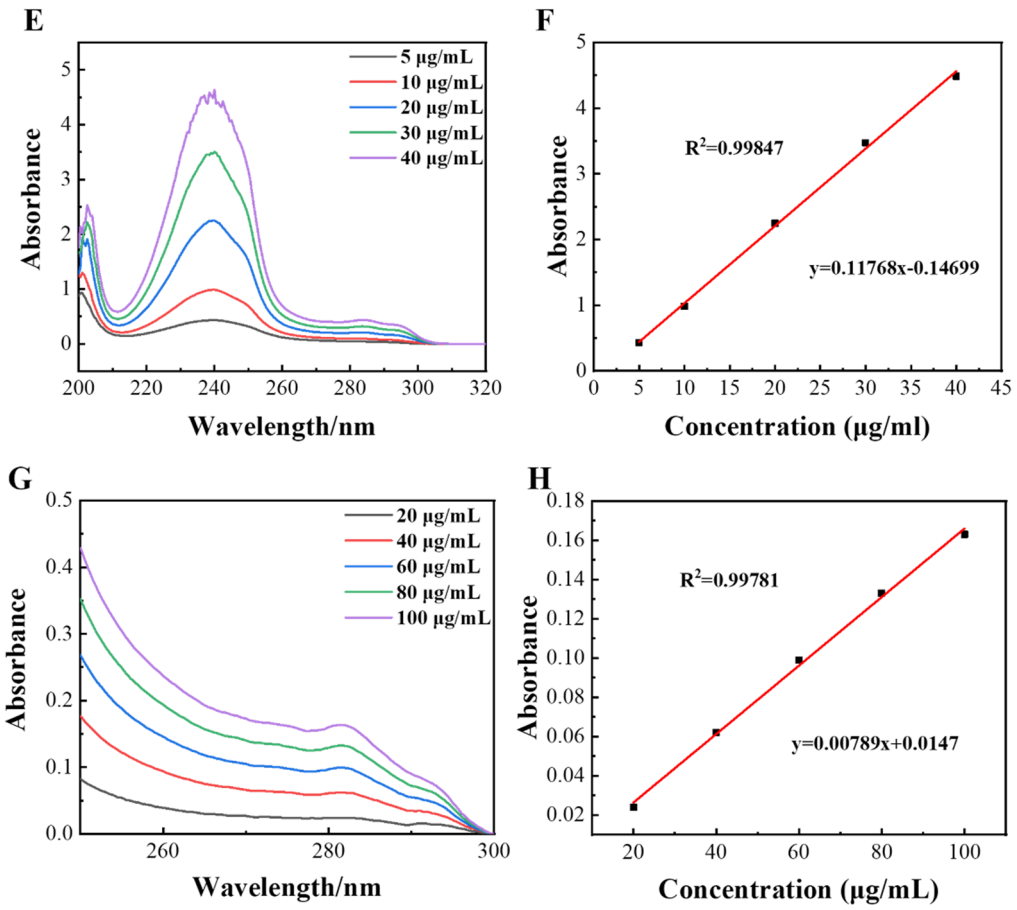


Figure S6. A) UV-Vis spectra of different concentration of PA solution. B) The linear relationship between the concentration and UV-Vis absorbance of PA solution. C) UV-Vis spectra of different concentration of IPA solution. D) The linear relationship between the concentration and UV-Vis absorbance of IPA solution. E) UV-Vis spectra of different concentration of TPA solution. F) The linear relationship between the concentration and UV-Vis absorbance of TPA solution. G) UV-Vis spectra of different concentration of TA solution. H) The linear relationship between the concentration and UV-Vis absorbance of TA solution.

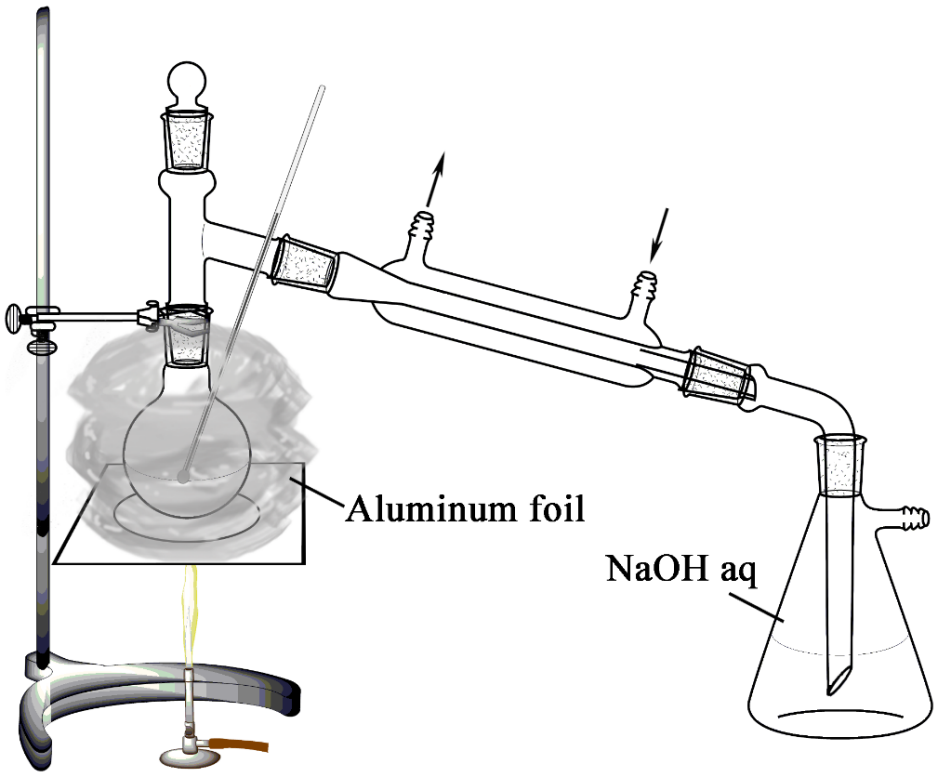


Figure S7. The system to collect the sublimated PA.

Table S1. Quantitative determination of the benzoic acid derivatives' content in BADs@BA by UV-Vis spectra.

Samples	Absorbance	Average of absorbance	Theoretical content (mg)	Sublimation content (mg)	Actual content (mg)	Content percentage
PA@BA	1.228	1.192	76.809	2.874	80.000	99.604%
	1.055					
	1.293					
IPA@BA	0.674	0.725	80.999		80.000	101.249%
	0.759					
	0.743					
TPA@BA	2.302	2.475	79.348		80.000	99.184%
	2.587					
	2.537					
TA@BA	0.032	0.035	78.516		80.000	98.146%
	0.039					
	0.034					

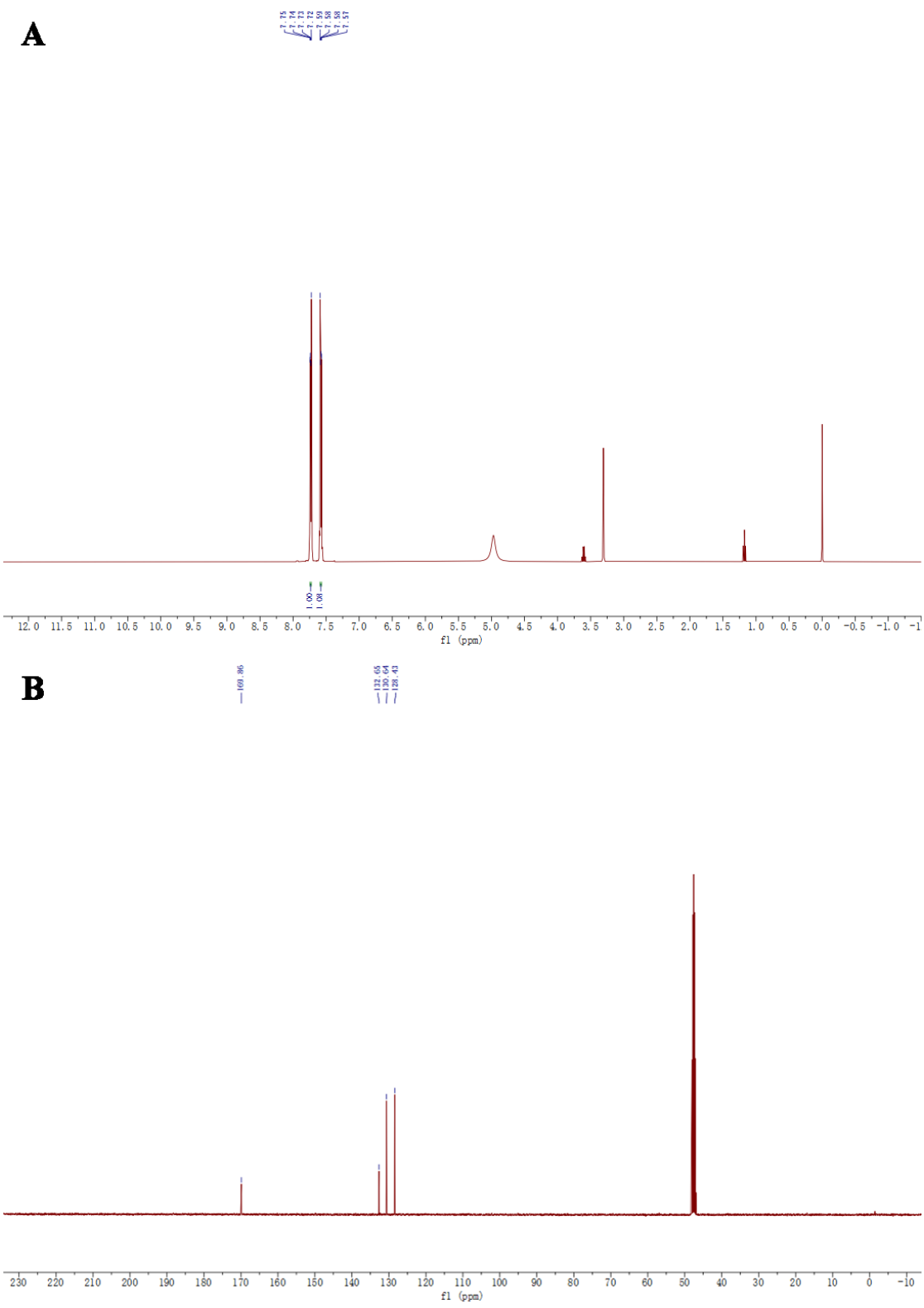


Figure S8. A) ^{1}H NMR spectrum of the PA@BA sublimation: ^{1}H NMR (400 MHz, D_2O) δ 7.73 (dd, J=4, 8 Hz, 2H), 7.58 (dd, J=4, 8 Hz, 2H). B) ^{13}C NMR spectrum of the PA@BA sublimation: ^{13}C NMR (400 MHz, D_2O) δ 169.86, 132.65, 130.64, 128.43.

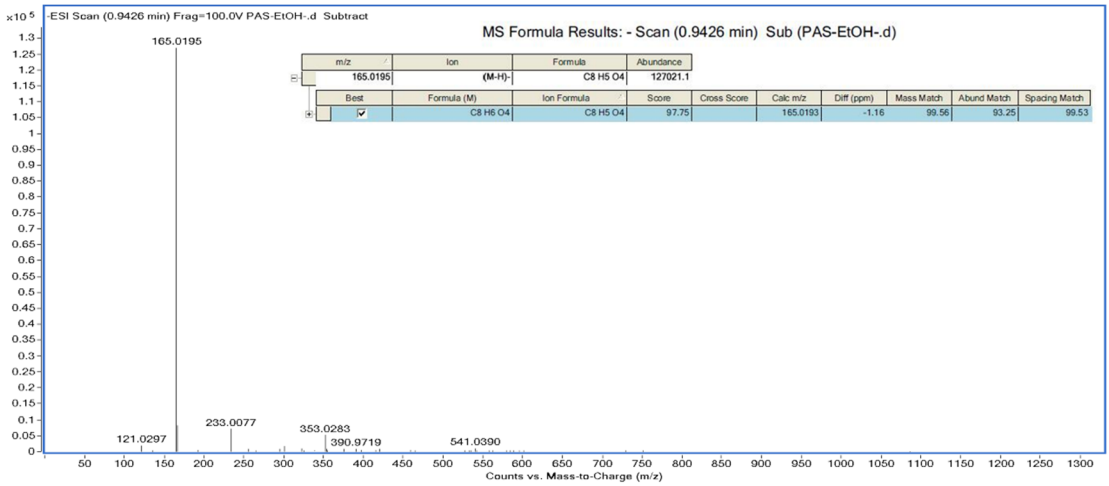
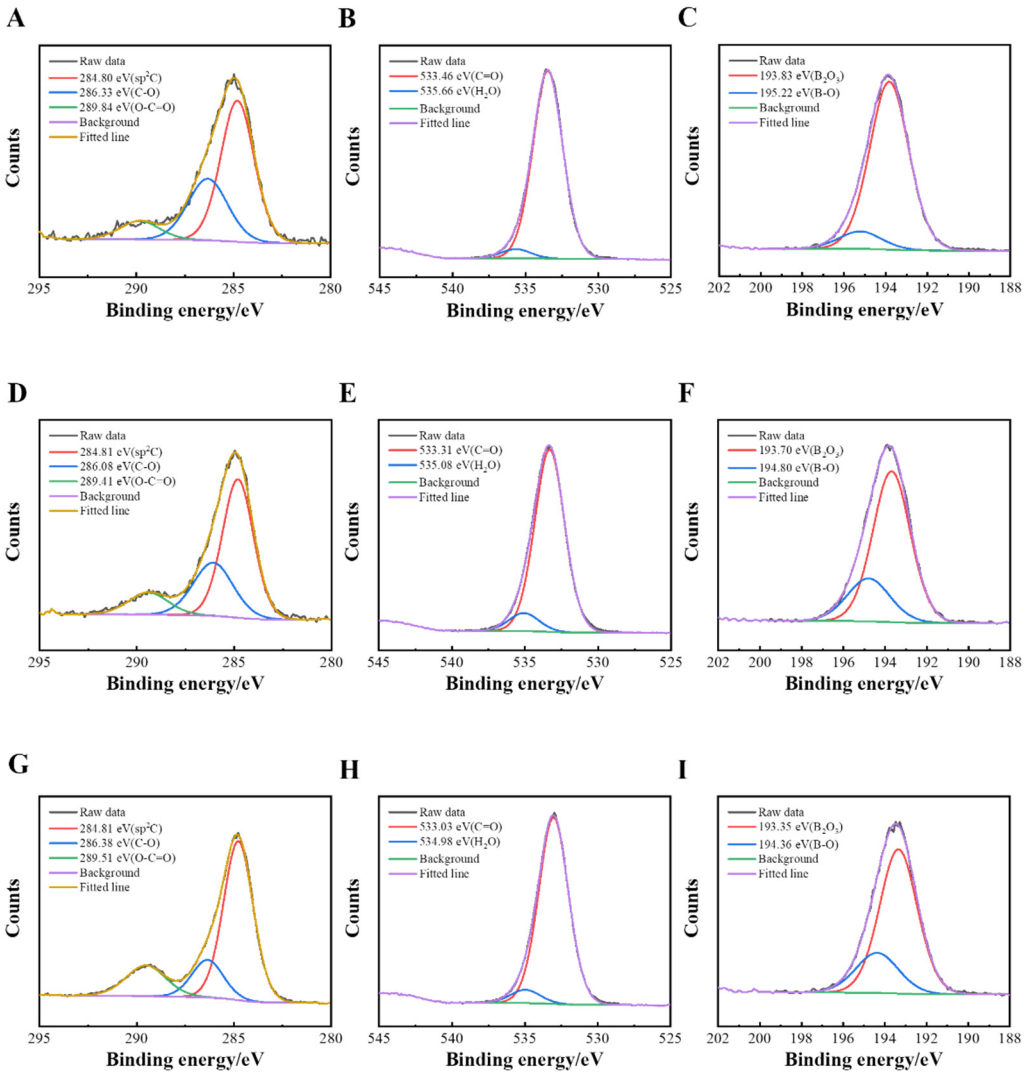


Figure S9. Mass spectrum of the PA@BA sublimation



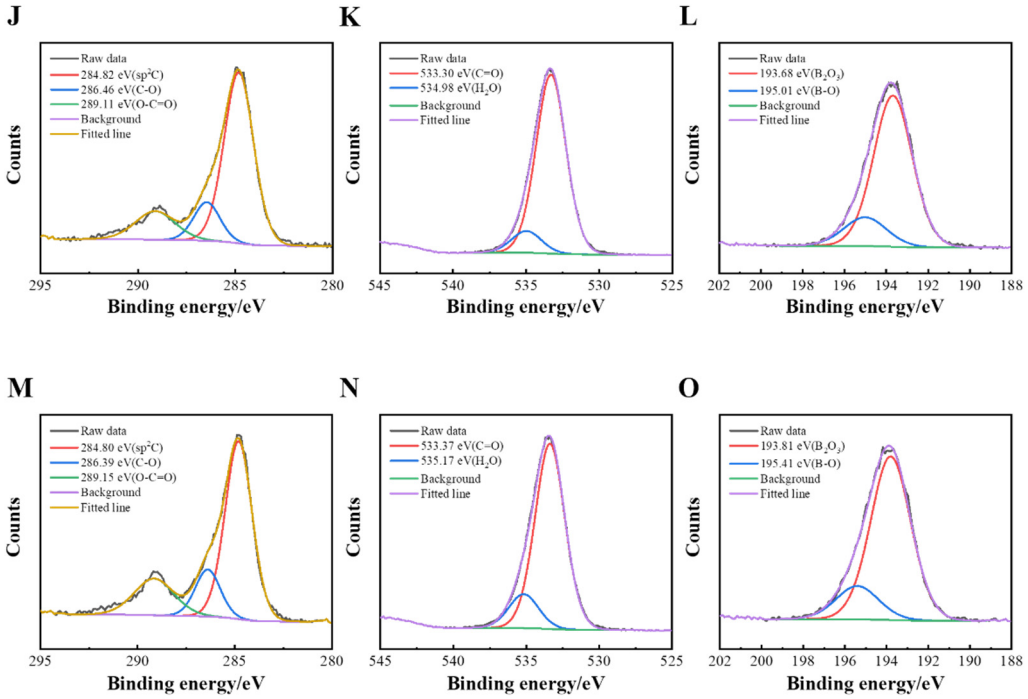
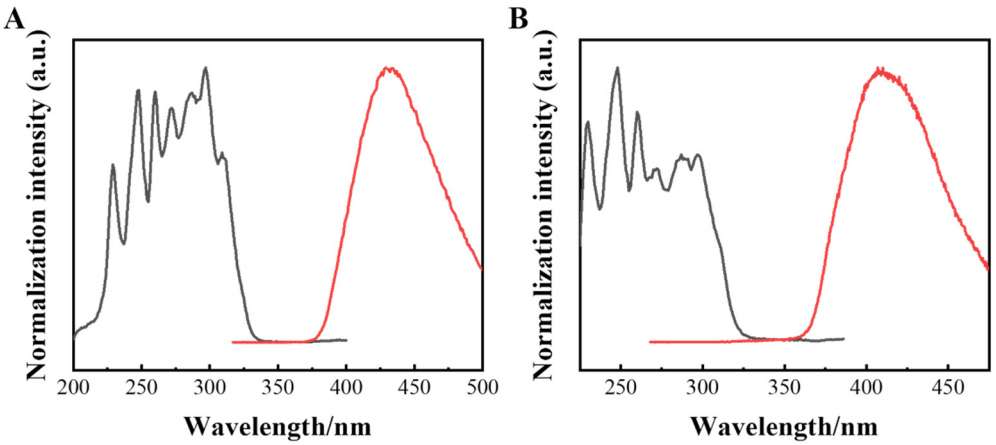


Figure S10. A), B) and C) XPS high-resolution C 1s, O 1s and B 1s spectra of BA, respectively. D), E) and F) XPS high-resolution C 1s, O 1s and B 1s spectra of PA@BA, respectively. G), H) and I) XPS high-resolution C 1s, O 1s and B 1s spectra of IPA@BA, respectively. J), K) and L) XPS high-resolution C 1s, O 1s and B 1s spectra of TPA@BA, respectively. M), N) and O) XPS high-resolution C 1s, O 1s and B 1s spectra of TA@BA, respectively.

II. Photophysical properties of BADs@BA



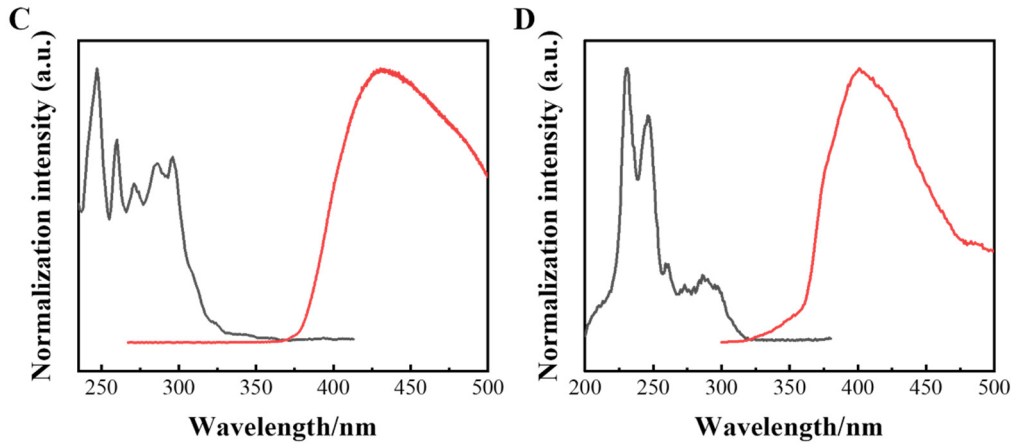


Figure S11. A) The phosphorescence excitation and emission spectra of PA@BA. B) The phosphorescence excitation and emission spectra of IPA@BA. C) The phosphorescence excitation and emission spectra of TPA@BA. D) The phosphorescence excitation and emission spectra of TA@BA.

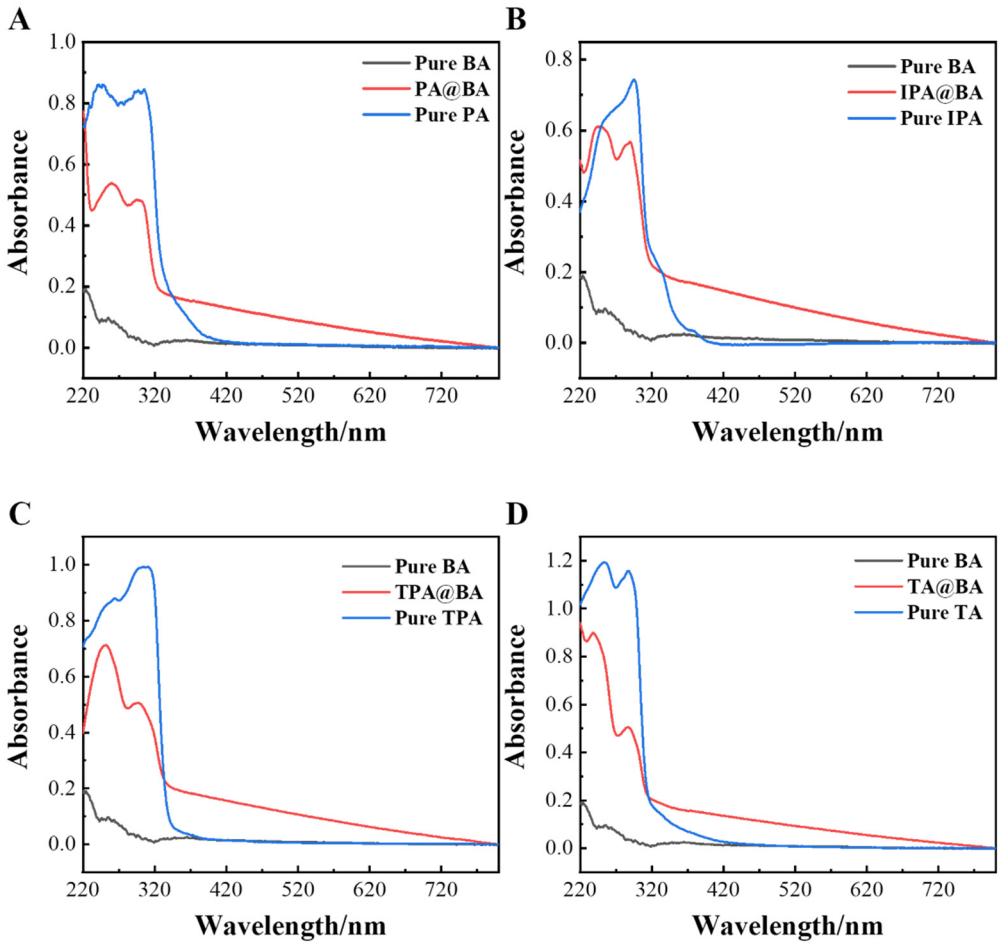


Figure S12. A) The solid-state UV-Vis spectra of PA, PA@BADs and pure BA. B) The

solid-state UV-Vis spectra of IPA, IPA@BADs and pure BA. C) The solid-state UV-Vis spectra of TPA, TPA@BADs and pure BA. D) The solid-state UV-Vis spectra of TA, TA@BADs and pure BA.

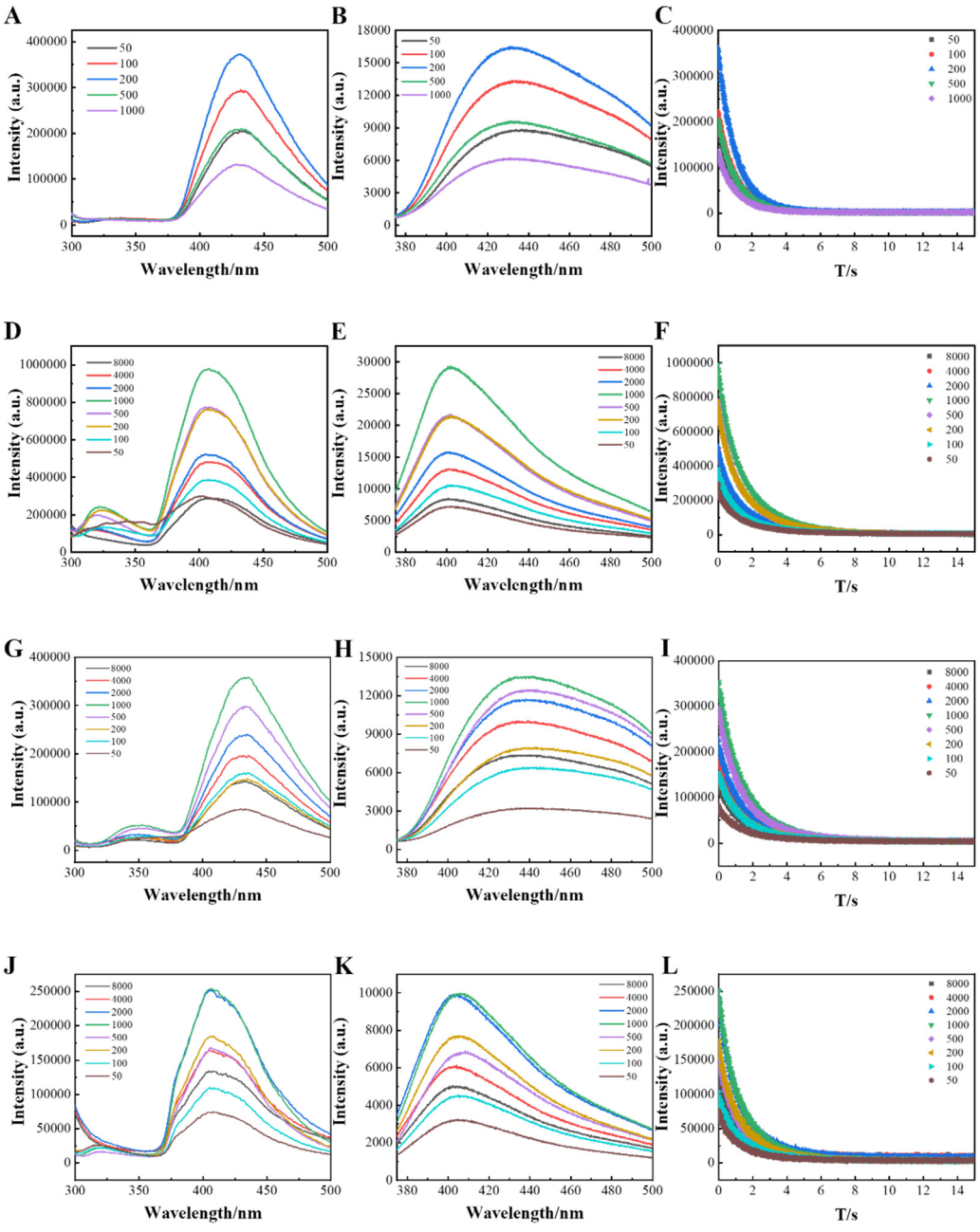


Figure S13. A), B) and C) fluorescence spectra, phosphorescence spectra and lifetime decay profiles of different ratio PA@BA under ambient conditions. D), E) and F) fluorescence spectra, phosphorescence spectra and lifetime decay profiles of different ratio IPA@BA under ambient conditions. G), H) and I) fluorescence spectra,

phosphorescence spectra and lifetime decay profiles of different ratio TPA@BA under ambient conditions. J), K) and L) fluorescence spectra, phosphorescence spectra and lifetime decay profiles of different ratio TA@BA under ambient conditions, respectively.

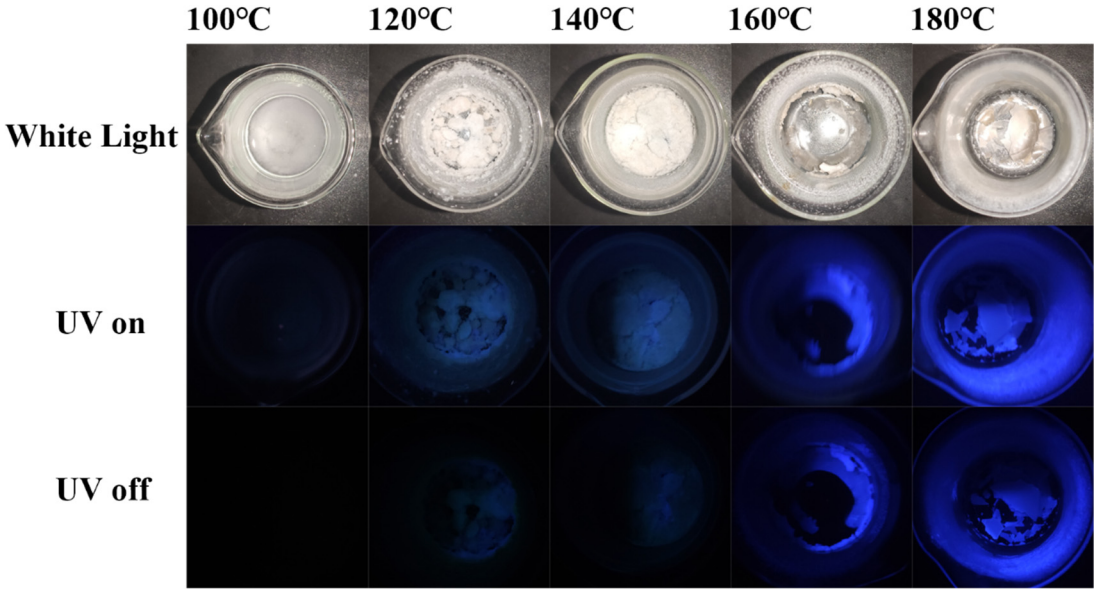


Figure S14. The different synthesized temperature of IPA@BA under white light and 254 nm handy UV lamp.

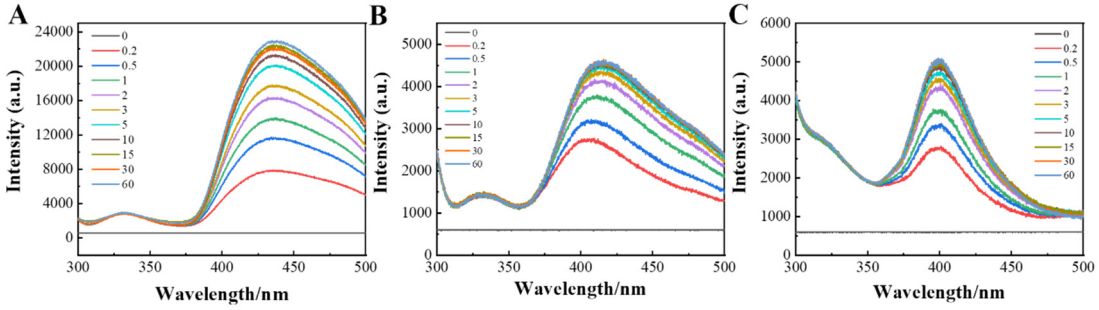


Figure S15. A) Fluorescence spectra of PA@BA excited at different seconds. B) Fluorescence spectra of TPA@BA excited at different seconds. C) Fluorescence spectra of TA@BA excited at different seconds.

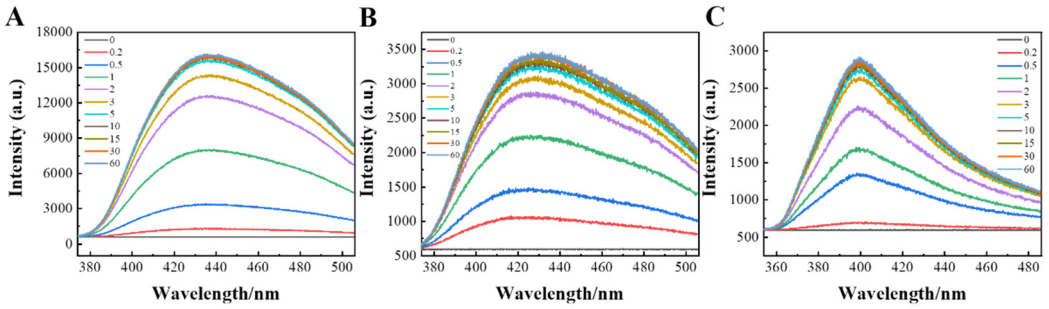


Figure S16. A) Phosphorescence spectra of PA@BA excited at different seconds. B) Phosphorescence spectra of TPA@BA excited at different seconds. C) Phosphorescence spectra of TA@BA excited at different seconds.

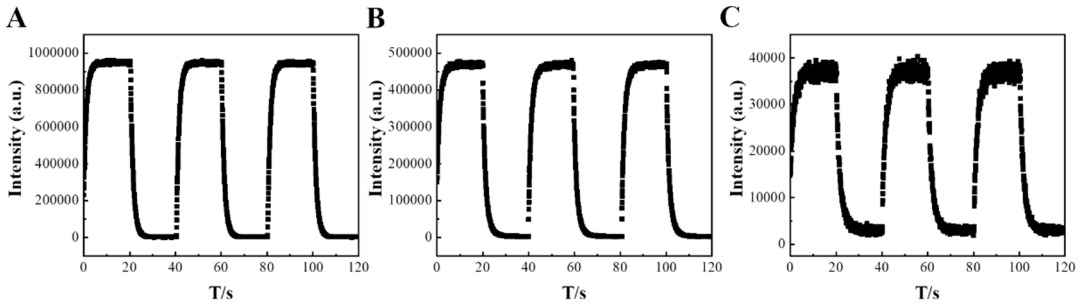


Figure S17. A) The cycle of PA@BA photo-activation and deactivation behavior during 120 seconds. B) The cycle of TPA@BA photo-activation and deactivation behavior during 120 seconds. C) The cycle of TA@BA photo-activation and deactivation behavior during 120 seconds.

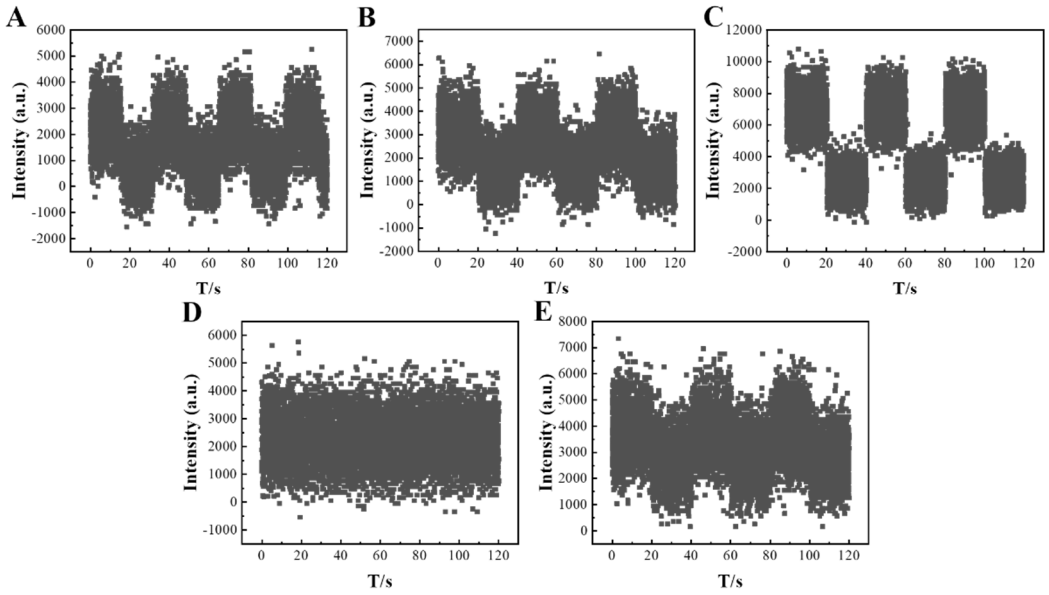


Figure S18. A) The cycle of pure BA during 120 seconds. B) The cycle of pure PA during 120 seconds. C) The cycle of pure IPA during 120 seconds. D) The cycle of pure TPA during 120 seconds. E) The cycle of pure TA during 120 seconds, respectively.

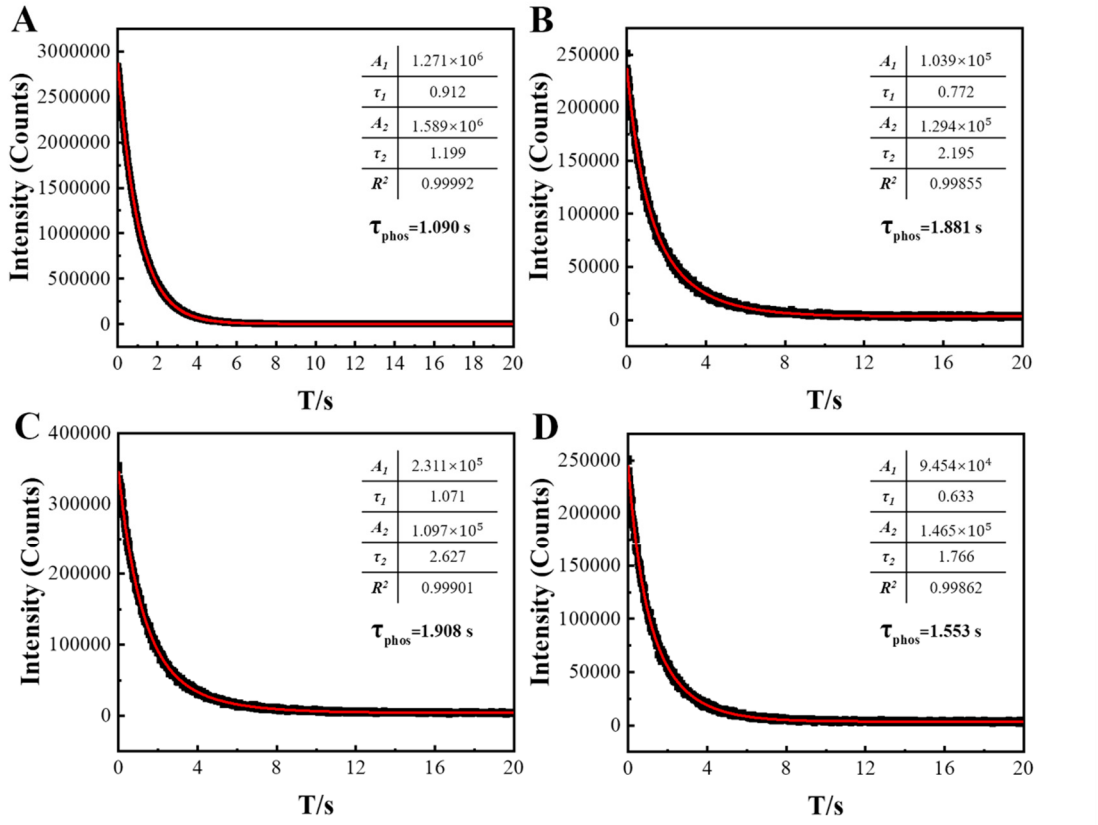


Figure S19. A) Lifetime decay profiles of PA@BA after photo-activation under ambient condition. B) Lifetime decay profiles of IPA@BA after photo-activation under ambient condition. C) Lifetime decay profiles of TPA@BA after photo-activation under

ambient condition. D) Lifetime decay profiles of TA@BA after photo-activation under ambient condition, respectively.

Table S2. The phosphorescence quantum yield of BADs@BA after photoactivated by excitation light.

Sample	λ_{ex}/nm	λ_f/nm	λ_p/nm	τ_p/s	Φ_p
PA@BA	297	332	434	1.071	47.52%
IPA@BA	248	328	404	1.881	38.79%
TPA@BA	247	340	429	1.908	66.98%
TA@BA	230	320	401	1.553	39.58%

III. The effect of time, power, temperature and atmosphere on URTP-PSR

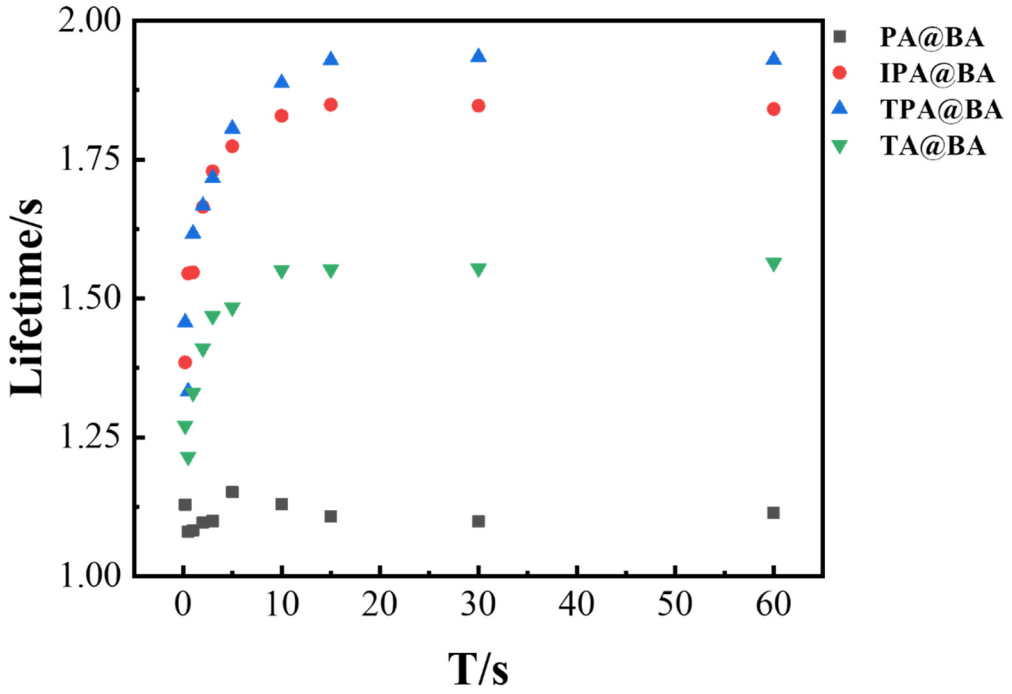


Figure S20. The lifetimes of BADs@BA after different photo-activated times ranging from 0.2 to 60 seconds under ambient conditions.

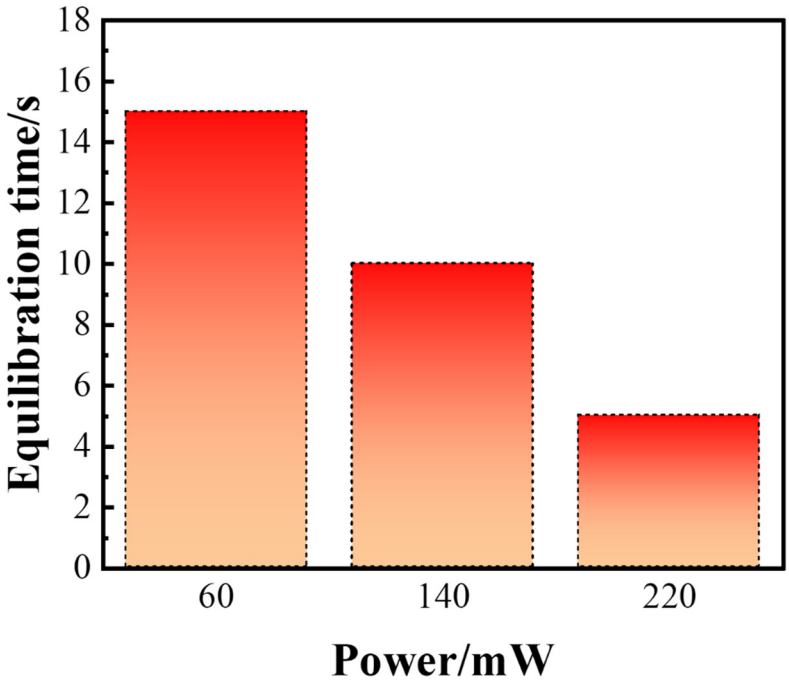


Figure S21. The equilibration photo-activation time of BADs@BA under different excitation power.

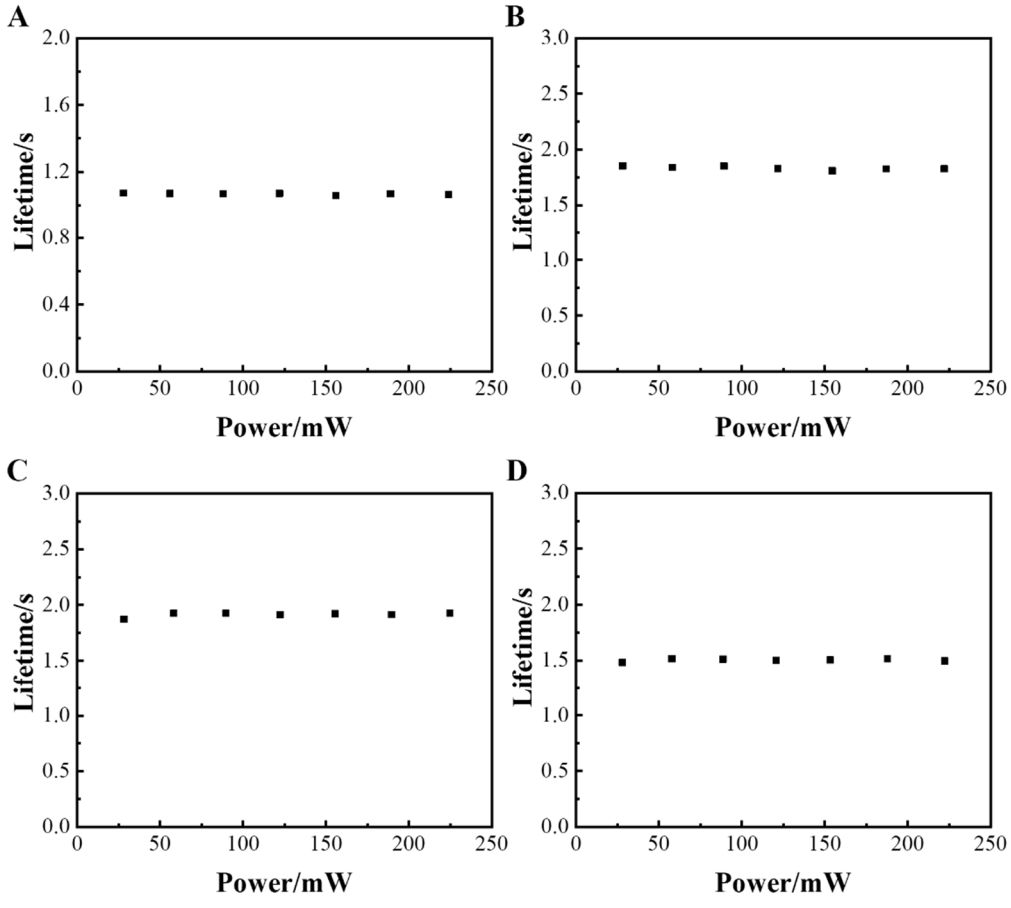


Figure S22. A) The lifetimes of PA@BA under different excitation light power. B) The

lifetimes of IPA@BA under different excitation light power. C) The photo-activation lifetimes of TPA@BA under different excitation light power. D) the lifetimes of TA@BA under different excitation light power, respectively.

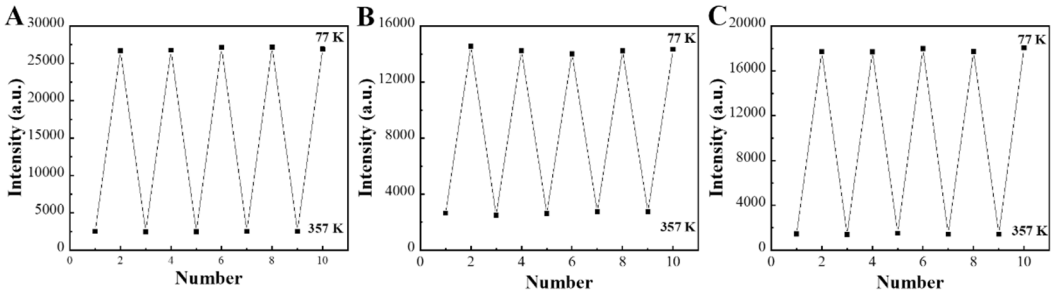


Figure S23. A) The temperature cyclicality of PA@BA between 77 K and 357 K. B) The temperature cyclicality of TPA@BA between 77 K and 357 K. C) The temperature cyclicality of TA@BA between 77 K and 357 K.

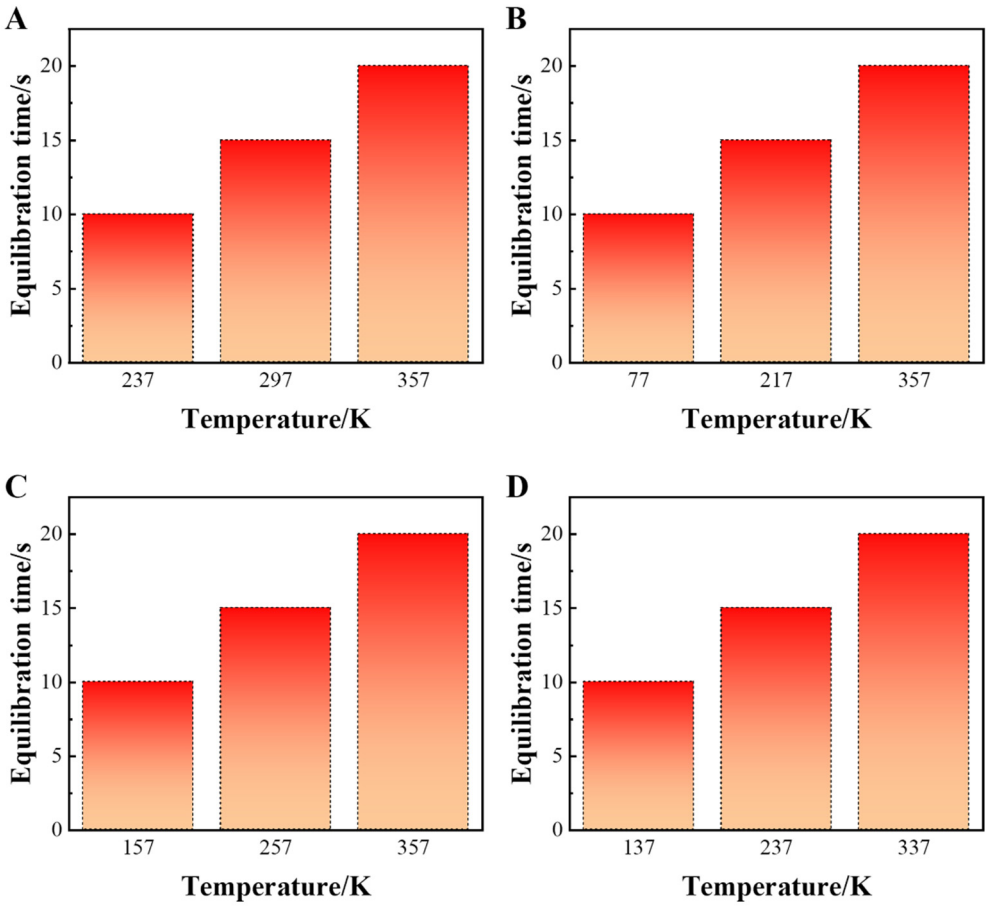
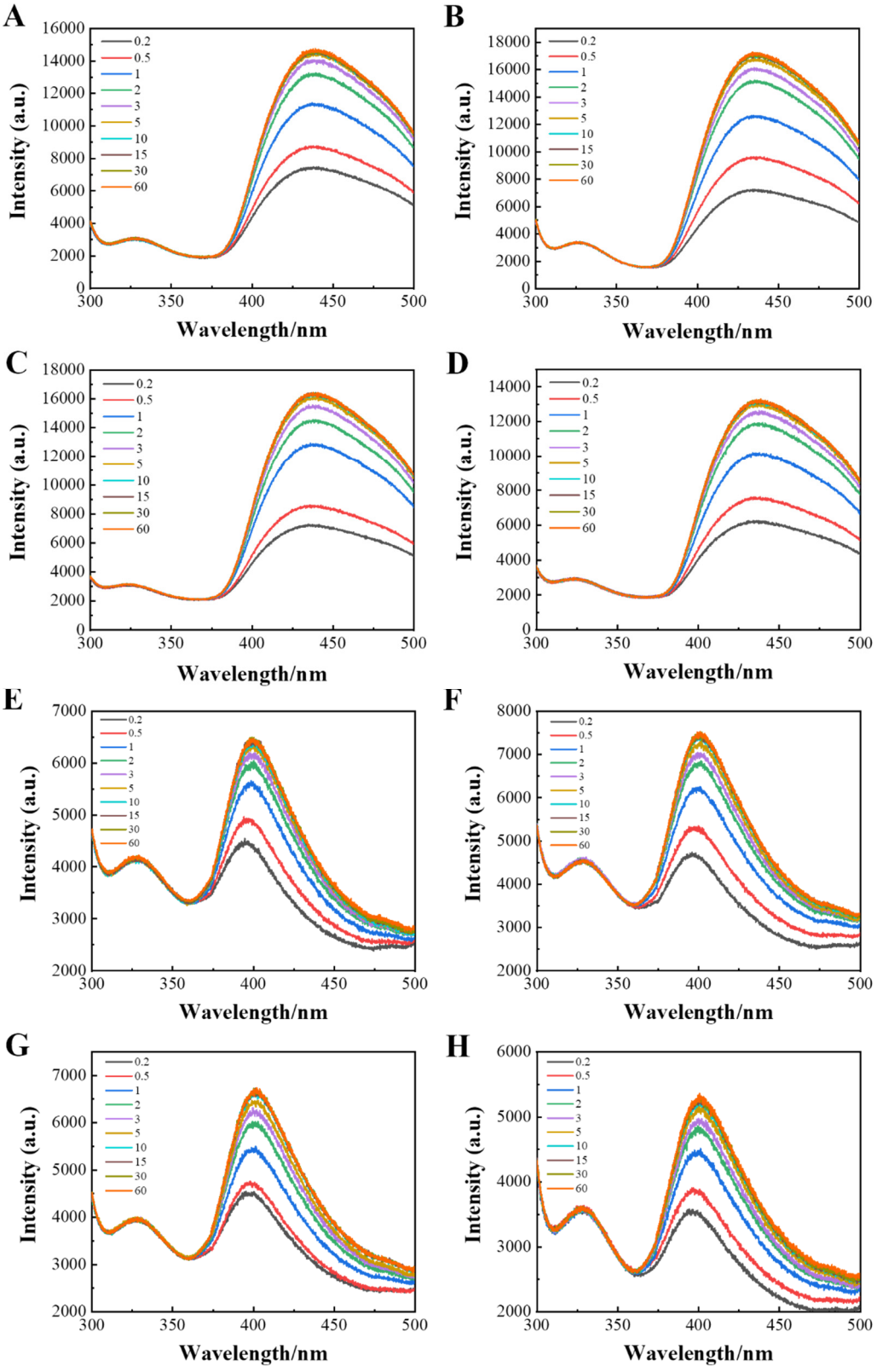


Figure S24. A) The equilibration photo-activation time of PA@BA under different temperature. B) The equilibration photo-activation time of IPA@BA under different

temperature. C) The equilibration photo-activation time of TPA@BA under different temperature. D) The equilibration photo-activation time of TA@BA under different temperature, respectively.



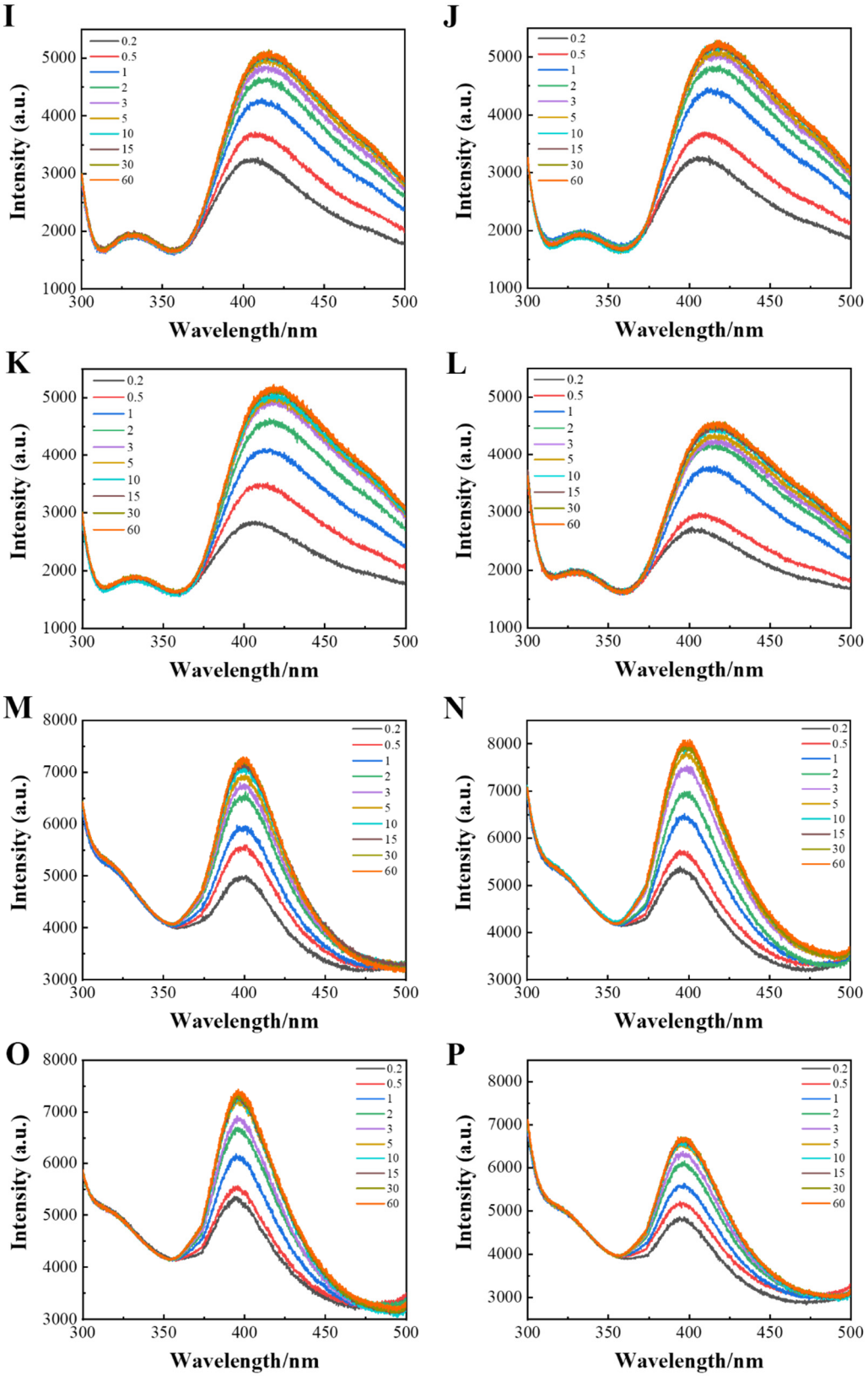


Figure S25. A), B), C) and D) fluorescence spectra of PA@BA under ambient, vacuum, nitrogen and oxygen atmosphere. E), F), G) and H) fluorescence spectra of IPA@BA under ambient, vacuum, nitrogen and oxygen atmosphere. I), J), K) and L) fluorescence

spectra of TPA@BA under ambient, vacuum, nitrogen and oxygen atmosphere. M), N), O) and P) fluorescence spectra of TA@BA under ambient, vacuum, nitrogen and oxygen atmosphere, respectively.

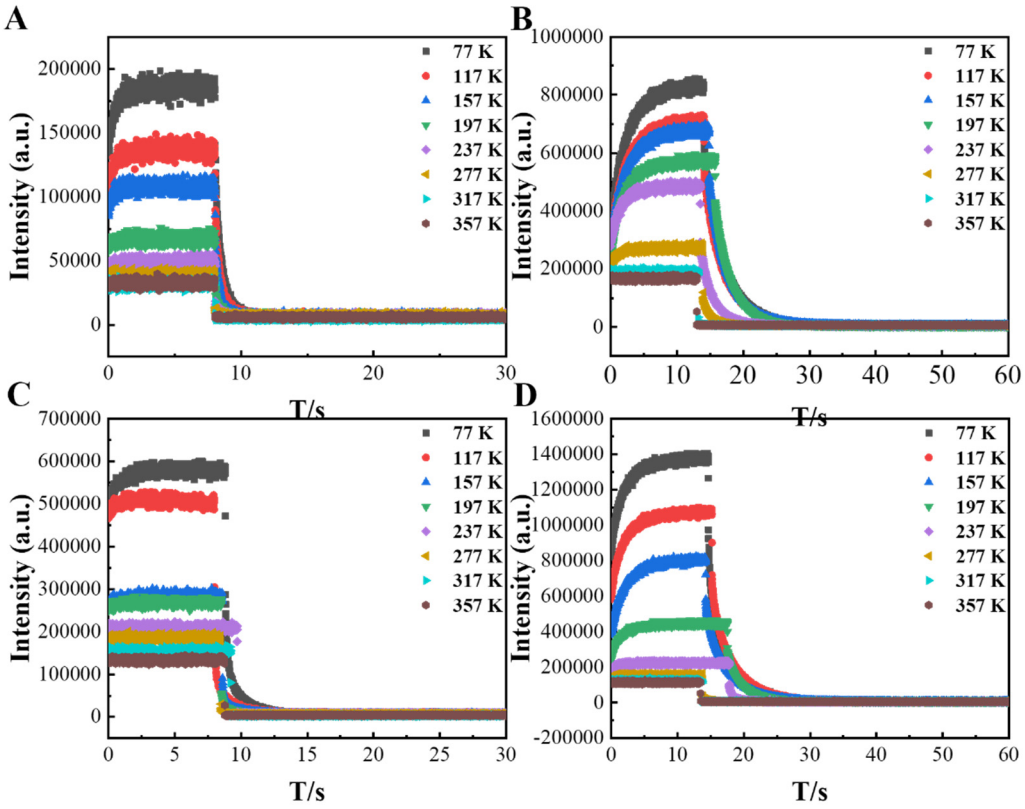


Figure S26. A) The photo-activation process of pure PA under different temperature. B) The photo-activation process of pure IPA under different temperature. C) The photo-activation process of pure TPA under different temperature. D) The photo-activation process of pure TA under different temperature, respectively.

IV. Theoretical calculations

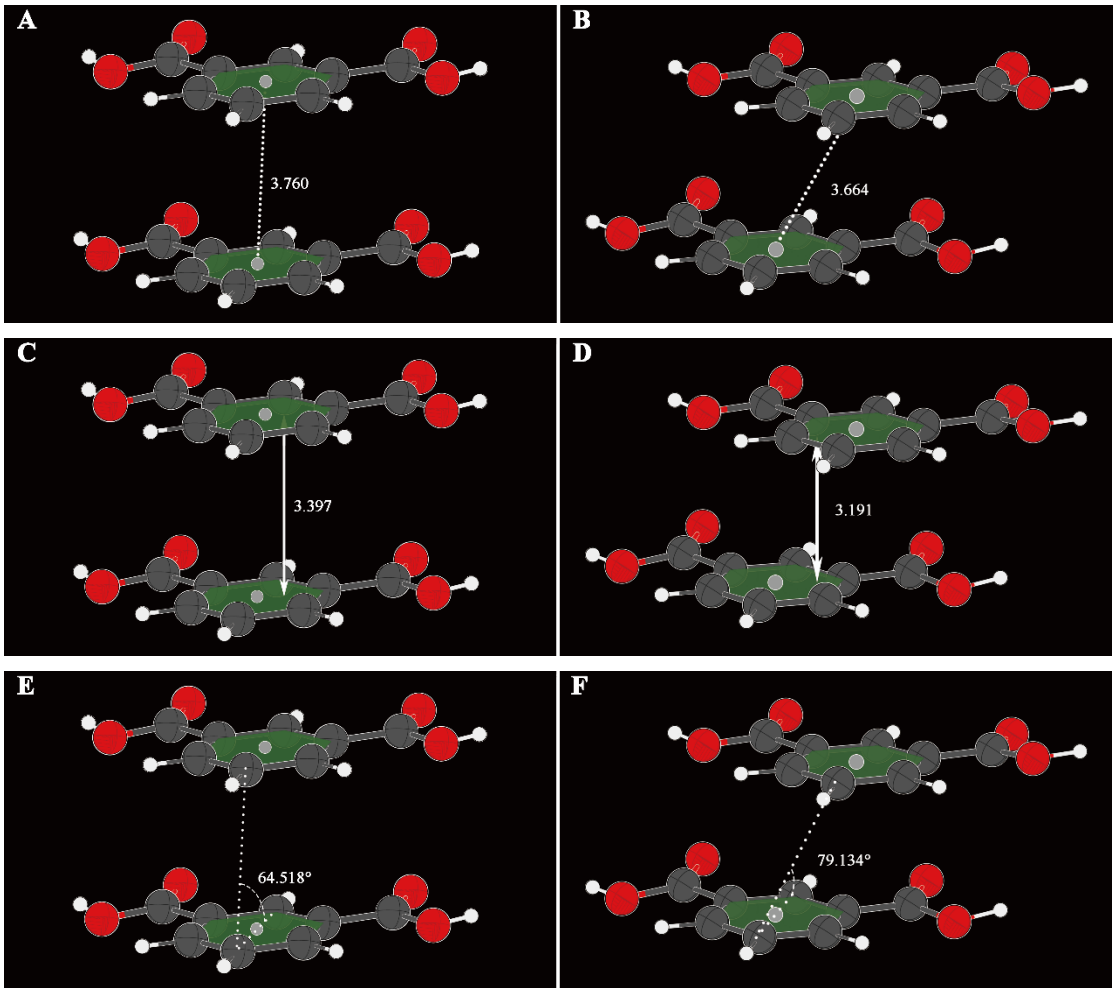


Figure S27. Molecular packing modes of IPA before photo-activation (from CIF) and after photo-activation (from TD-DFT calculating bas). A) Plane centroid to plane centroid distance of IPA before photo-activation. B) Plane centroid to plane centroid distance of IPA after photo-activation. C) Plane to plane distance of IPA before photo-activation. D) Plane to plane distance of IPA after photo-activation. E) The slip angle between π-stacked molecules of IPA before photo-activation. F) The slip angle between π-stacked molecules of IPA after photo-activation, respectively.

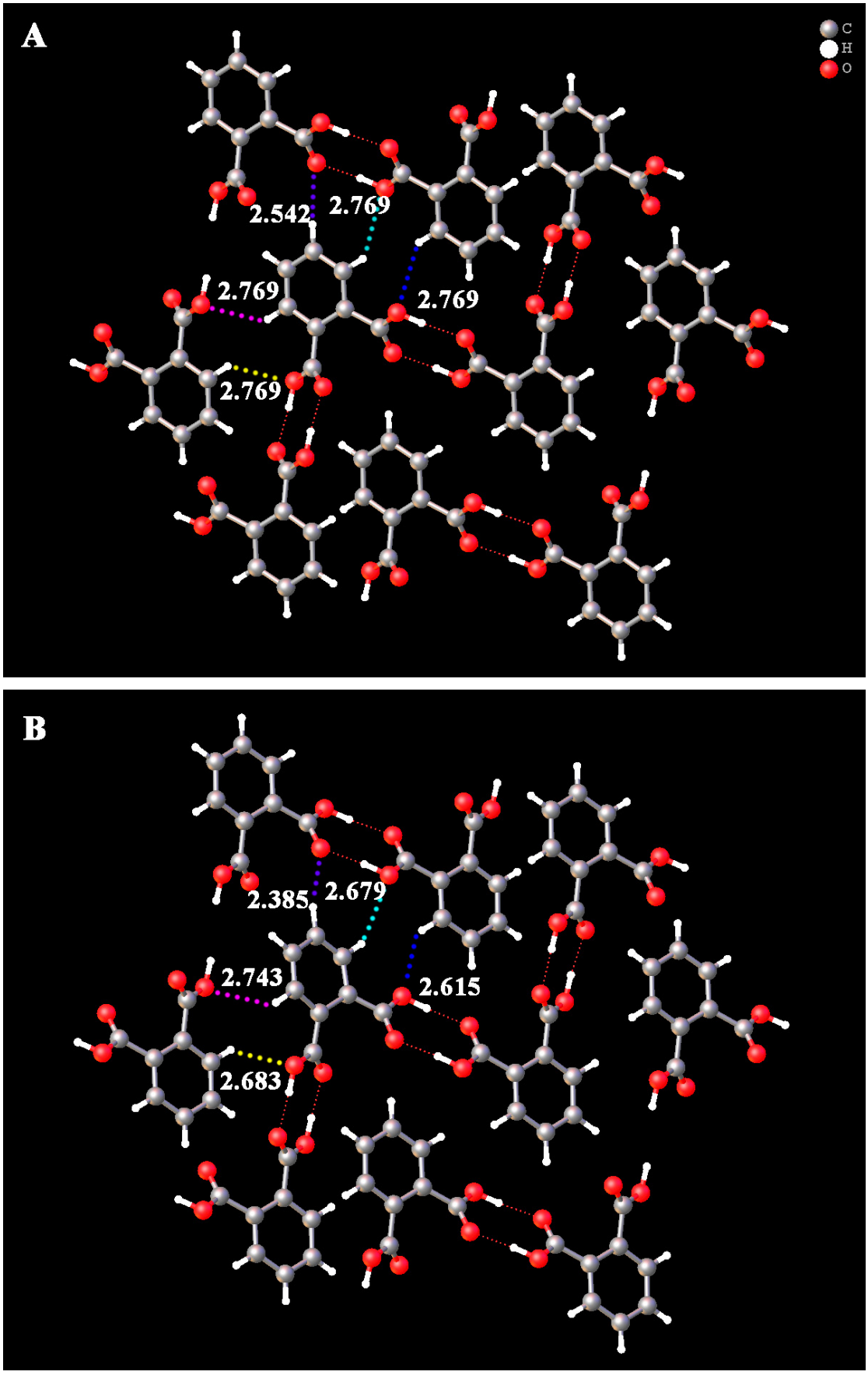


Figure S28. A) The distances of intermolecular interactions between two adjacent PA

molecules before photo-activation (from CIF). B) The distances of intermolecular interactions between two adjacent PA molecules after photo-activation (from TD-DFT calculating).

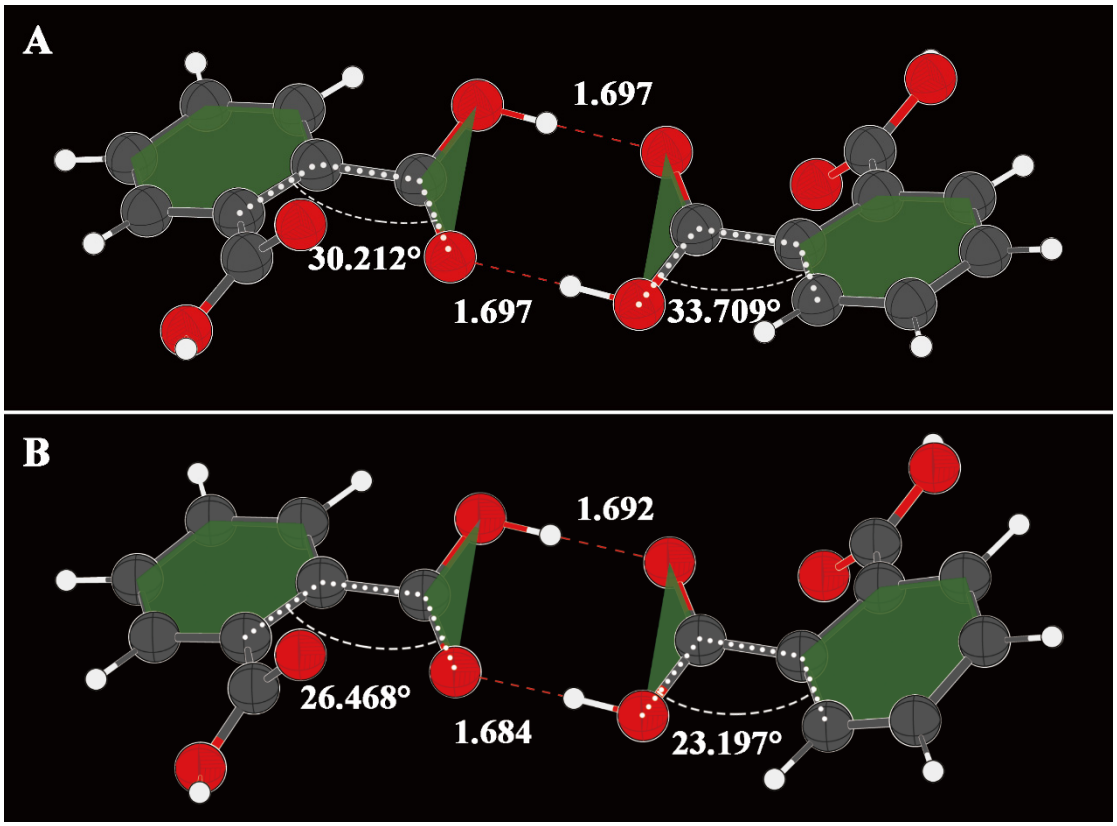


Figure S29 A) Intermolecular interactions and twisting angles of PA before photo-activation by single crystal. B) Intermolecular interactions and twisting angles of PA after photo-activation by calculating.

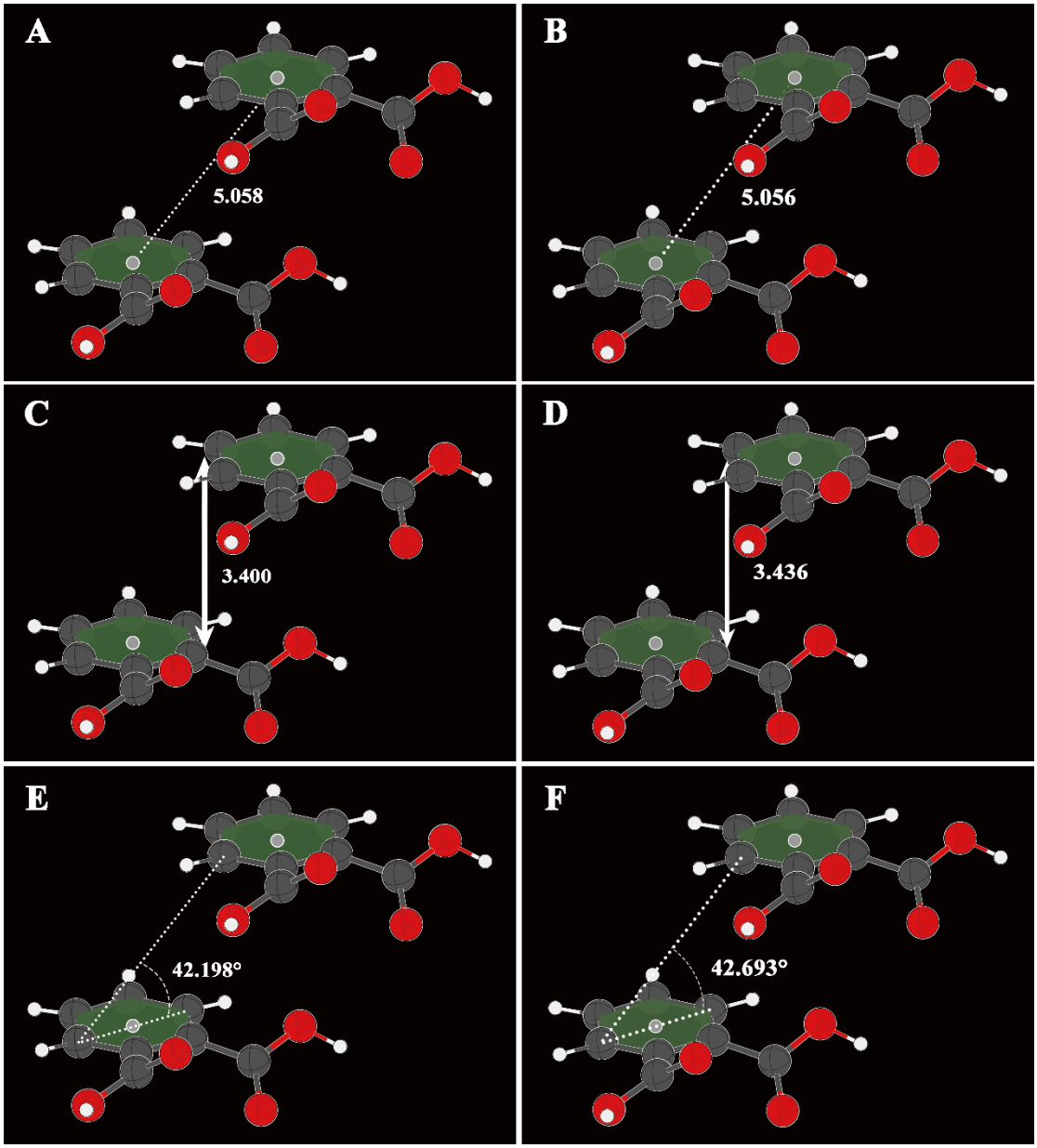


Figure S30. Molecular packing modes of PA before photo-activation (from CIF) and after photo-activation (from TD-DFT calculating). A) Plane centroid to plane centroid distance of PA before photo-activation. B) Plane centroid to plane centroid distance of PA after photo-activation. C) Plane to plane distance of PA before photo-activation. D) Plane to plane distance of PA after photo-activation. E) The slip angle between π-stacked molecules of PA before photo-activation. F) The slip angle between π-stacked molecules of PA after photo-activation, respectively.

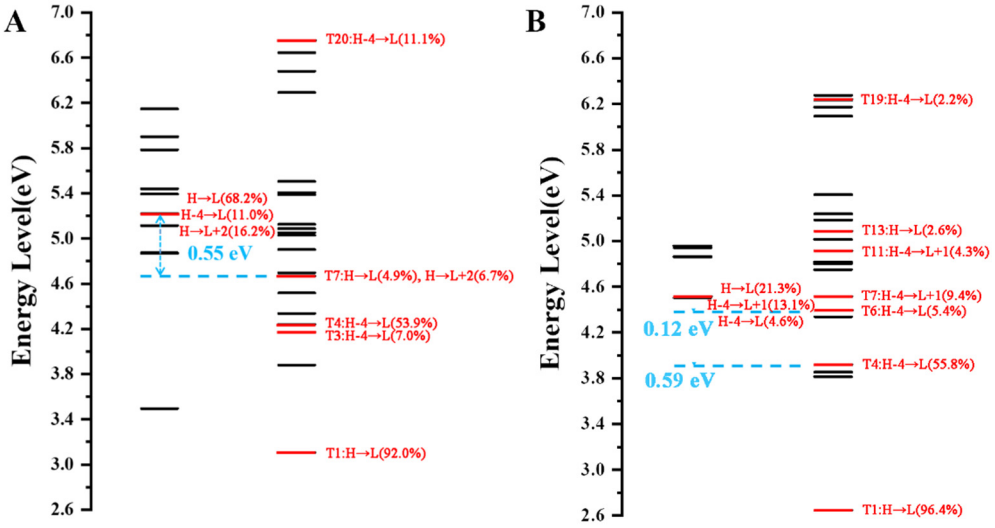


Figure S31. A) The TD-DFT-calculated excited-state energy levels and possible ISC channels of IPA. B) The TD-DFT-calculated excited-state energy levels and possible ISC channels of PA.

V. Research of BADs@PMMA

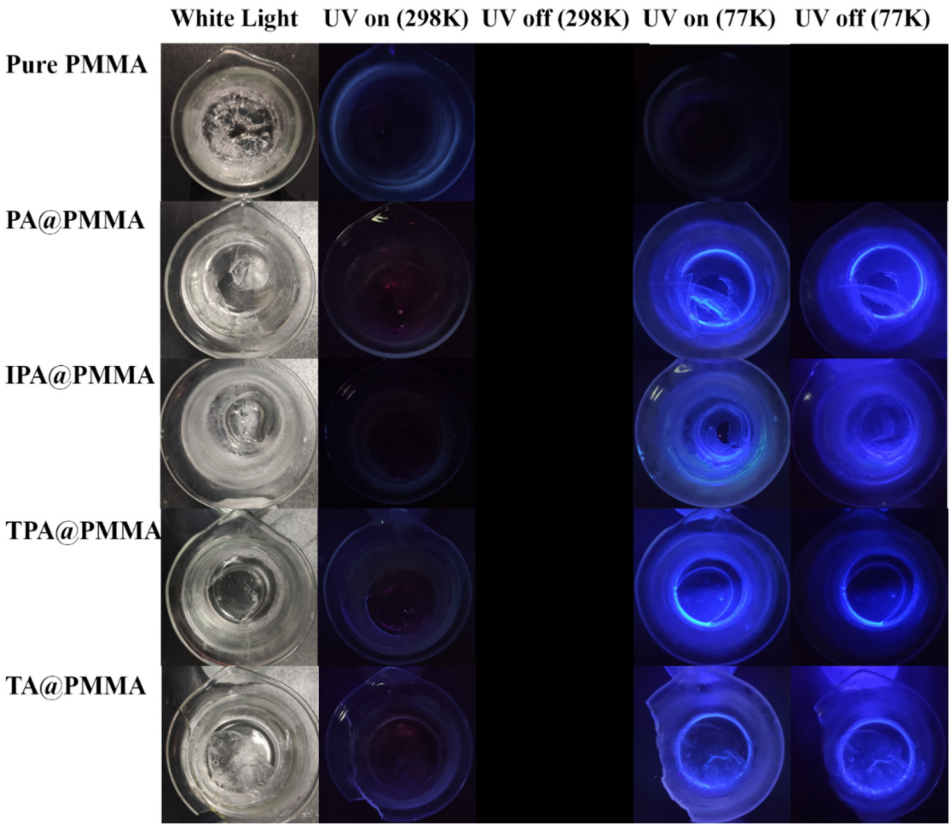


Figure S32. The photo of BADs@PMMA under white light and 254 nm handy UV lamp in 298 K and 77 K conditions.

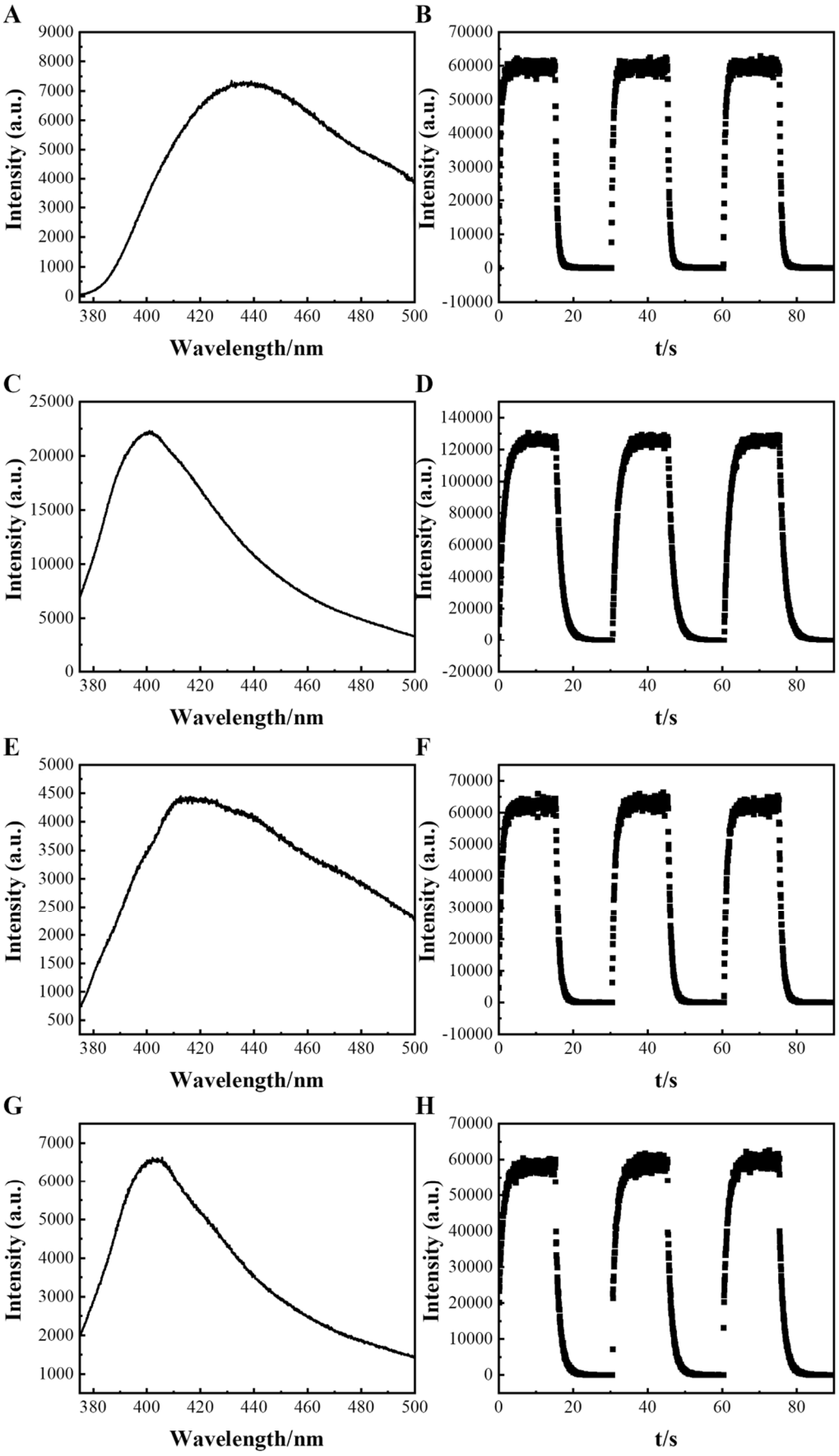


Figure S33. A) and B) the phosphorescence spectrum and photo-activation cycle of

PA@BA. C) and D) the phosphorescence spectrum and photo-activation cycle of IPA@BA. E) and F) the phosphorescence spectrum and photo-activation cycle of TPA@BA. G) and H) the phosphorescence spectrum and photo-activation cycle of TA@BA.