

Supporting Information

Continuous Tunable Emission Based on the Molecular Aggregation of (2Z,2'Z)-2,2'-(1,4-phenylene)bis(3-(4-(dodecyloxy) phenyl)acrylonitrile

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Supplementary Figures

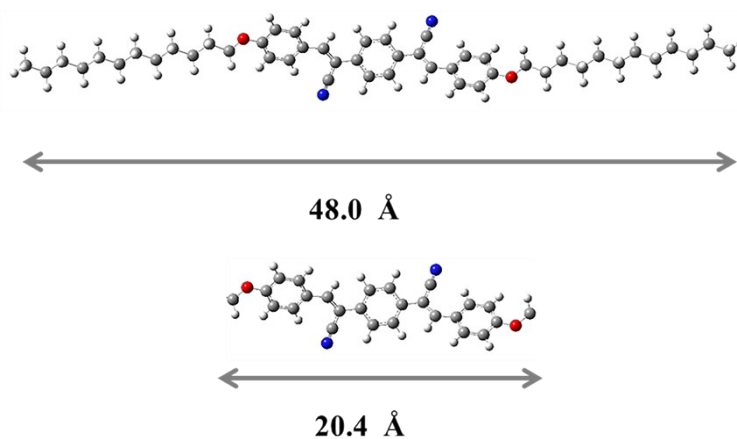


Fig. S1 Calculated optimized PDPA molecular structure.

Quantum Chemical Calculations: Single-molecule calculations in the gas phase were performed at the density functional theory (DFT) level of theory with the Gaussian 09 program. Herein, the ground-state geometry was fully optimized using the B3LYP functional and 3-21G basis set.

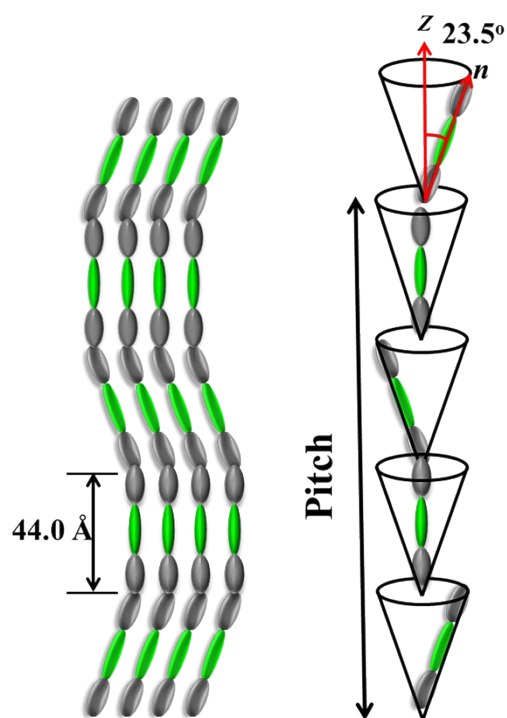


Fig. S2 Schematic illustration of the molecular arrangements in helical structure (phase I).

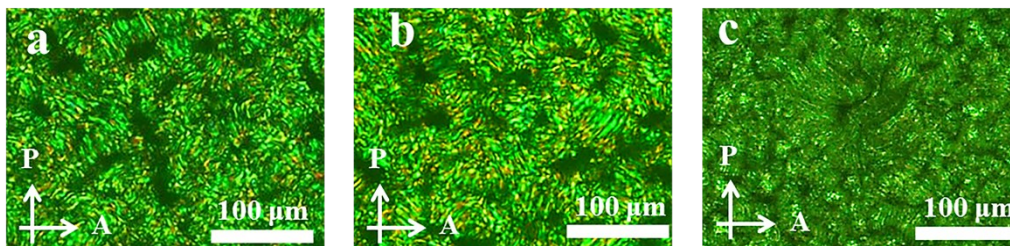


Fig. S3 PDPA POM images for cooling at 30 °C /min (a); at 40 °C /min (b); and at 50 °C /min (c).

Table S1. Fluorescence quantum yield of PDPA.

| Cooling rate(°C/min) | 0.5 | 5 | 10 | 20 | 30 | 40 | 50 |
|----------------------|--------|--------|--------|--------|--------|--------|--------|
| Absorb wavelength | 308 nm | 318 nm | 319 nm | 333 nm | 345 nm | 355 nm | 356 nm |
| Emission wavelength | 506 nm | 517 nm | 535 nm | 540 nm | 560 nm | 575 nm | 600 nm |
| QY | 26.37% | 50.18% | 54.26% | 55.9 % | 33.37% | 28.64% | 28.33% |

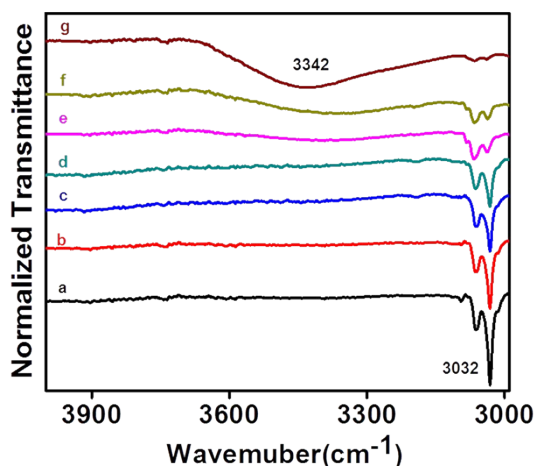


Fig. S4 PDPA IR spectra with different cooling rate:0.5 °C /min (a); 5 °C /min (b); 10 °C /min (c); 20 °C /min(d); 30 °C /min (e) ; 40 °C /min (f) ; and 50 °C /min (g).

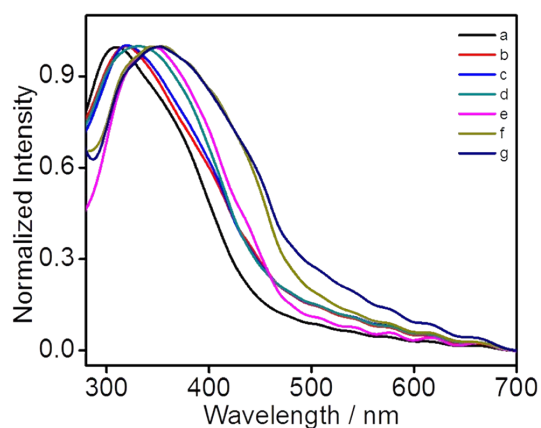


Fig. S5 PDPA UV absorption spectra with different cooling rate: at 0.5 °C /min (a); at 5 °C /min (b); at 10 °C /min (c); at 20 °C /min(d); at 30 °C /min (e); at 40 °C /min (f); and at 50 °C /min (g).

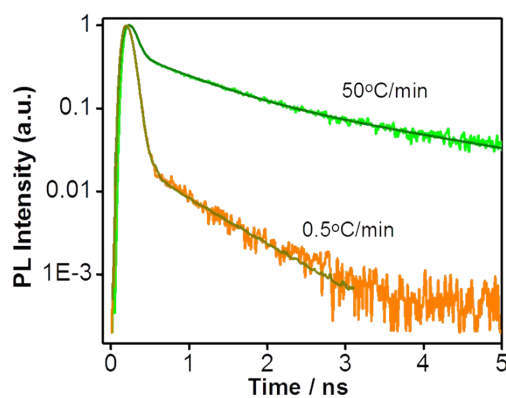


Fig. S6 Fluorescence decay profiles of PDPA film with the cooling rate ($0.5\text{ }^{\circ}\text{C min}^{-1}$ and $50\text{ }^{\circ}\text{C min}^{-1}$).

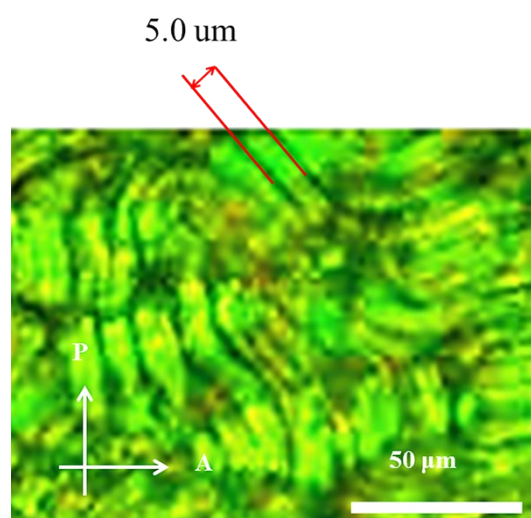


Fig. S7 The pitch length for the PDPA film with the cooling rate ($0.5\text{ }^{\circ}\text{C min}^{-1}$).