

Supporting Information

Morphology-controlled assembly and enhanced emission of fluorescence in organic nanospheres and microrods based on 1,2-diphenyl-4-(4-dibenzothienyl)phenyl)-1,3-cyclopentadiene

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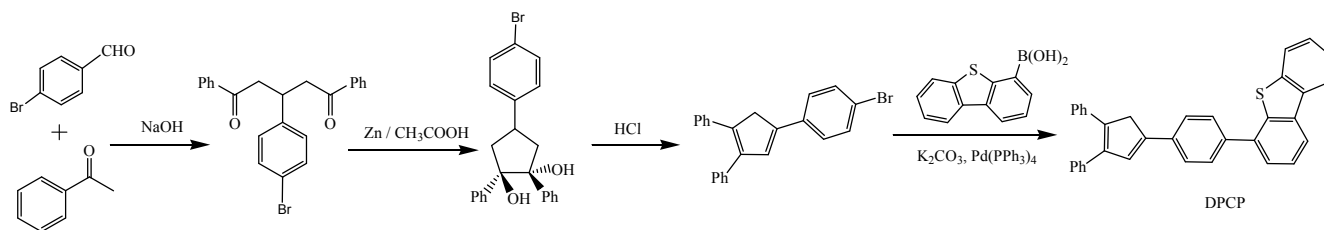
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Experiments

Synthesis of 1,2-diphenyl-4-(4-dibenzothiényl)phenyl)-1,3-cyclopentadiene (DPCP)

The synthetic route for DPCP and their chemical structures are shown in Scheme S1. 1,2-diphenyl-4-(4-bromophenyl)-1,3-diene was synthesized according to our previously work. 1,2-diphenyl-4-(4-bromophenyl)-1,3-diene (2.10 mmol) and the 4-dibenzothiénylboronic acid (2.40 mmol) in toluene (15 mL), 2 M aqueous K_2CO_3 solution (10 mL) and ethanol (5 mL) were added. The mixture was stirred for 30 min under an argon atmosphere at room temperature. Then the $Pd(PPh_3)_4$ catalyst was added and the reaction mixture was stirred at 80 °C for 24 h allowing the temperature to decrease gradually to room temperature. The crude product was concentrated and purified by silica gel column chromatography using petroleum ether/dichloromethane.

1H NMR (400 MHz, $CDCl_3$) δ (ppm): 8.23-8.21 (m, 1H), 8.19-8.17 (m, 1H), 7.88-7.86 (m, 1H), 7.79-7.74 (m, 4H), 7.59-7.57 (d, 1H), 7.56-7.54 (m, 1H), 7.51-7.49 (m, 2H), 7.46-7.44 (m, 2H), 7.39-7.34 (m, 5H), 7.32-7.29 (d, 1H), 7.27-7.25 (d, 1H), 7.22-7.21 (d, 1H), 7.16 (s, 1H), 4.04 (s, 2H).
 ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 144.5, 142.2, 139.7, 139.6, 139.1, 138.5, 137.2, 136.8, 136.7, 136.3, 135.8, 135.4, 132.4, 128.7, 128.6, 128.5, 128.3, 127.8, 127.3, 126.9, 126.8, 126.7, 125.3, 125.2, 124.4, 122.7, 121.8, 120.5, 45.0. MS (API-ES): calcd for $C_{35}H_{24}S$, M: 476.2. Elem. Anal.: C, 88.29%; H, 5.16%; S, 6.78%. Found: C, 88.20%; H, 5.08%; S, 6.73%.



Scheme S1

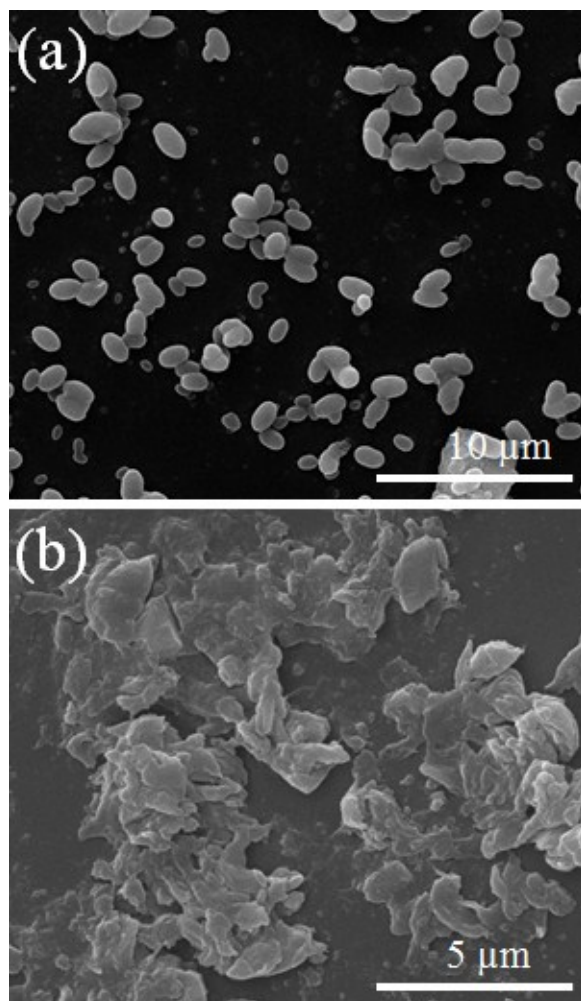


Fig. S1 SEM of DPCP particles obtained by using different solvents (a) ethanol and (b) tetrahydrofuran. Concentration: 0.01 mM.

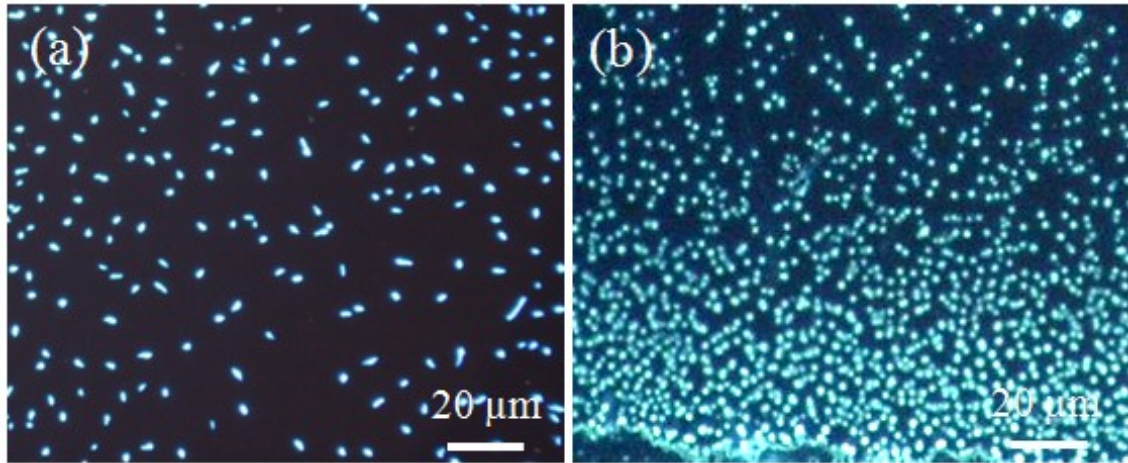


Fig. S2 FM images of DPCP particles prepared by using different surfactants (a) P123 and (b) CTAB.

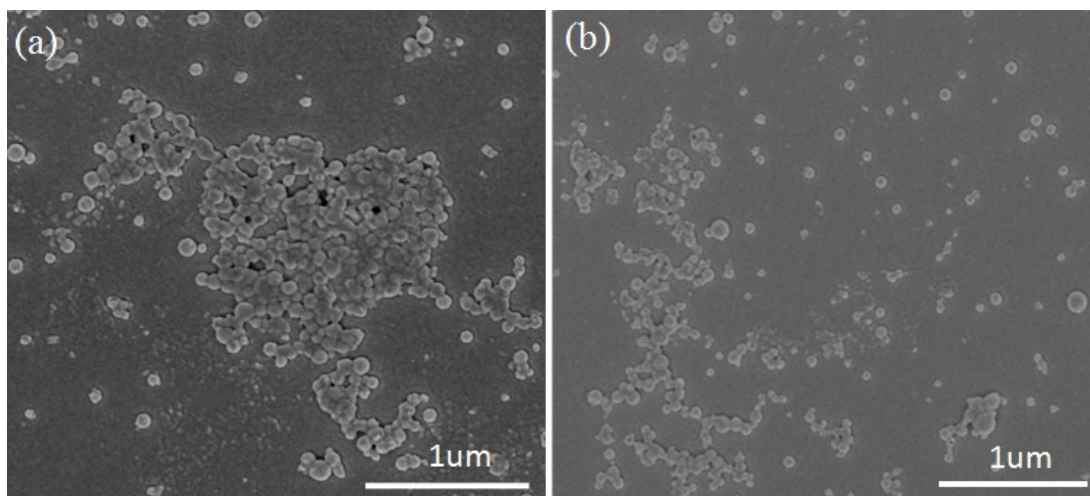


Fig. S3 SEM of DPCP particles obtained by using CTAB with different concentration (a) 0.5 mg/mL, (b) 1 mg/mL.

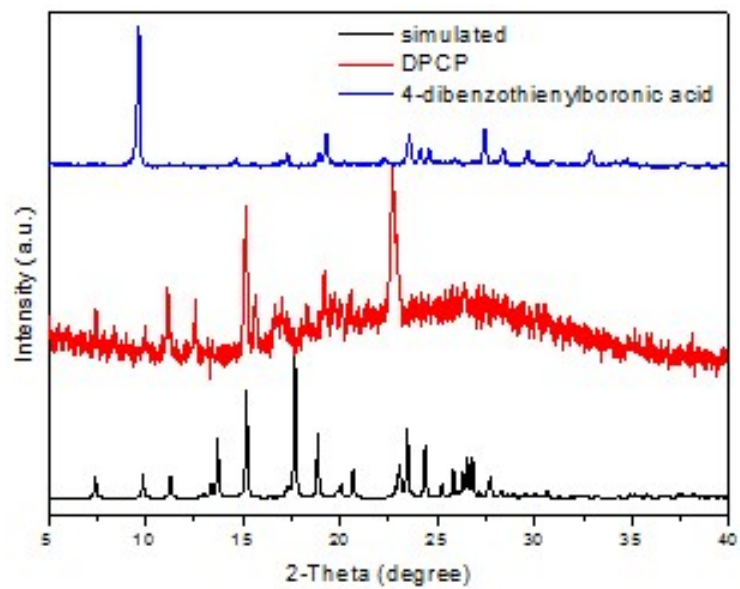


Fig. S4 PXR D patterns of 4-dibenzothienylboronic acid, simulated and experimental DPCP.

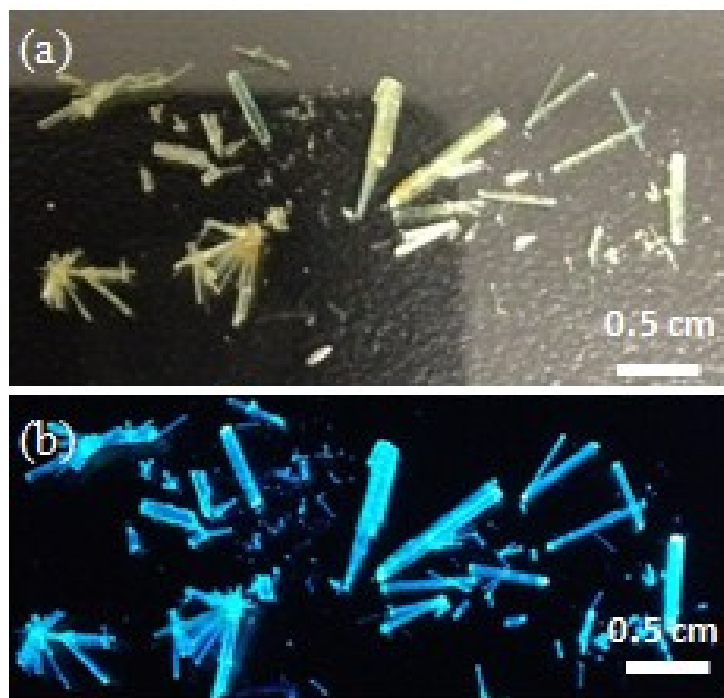
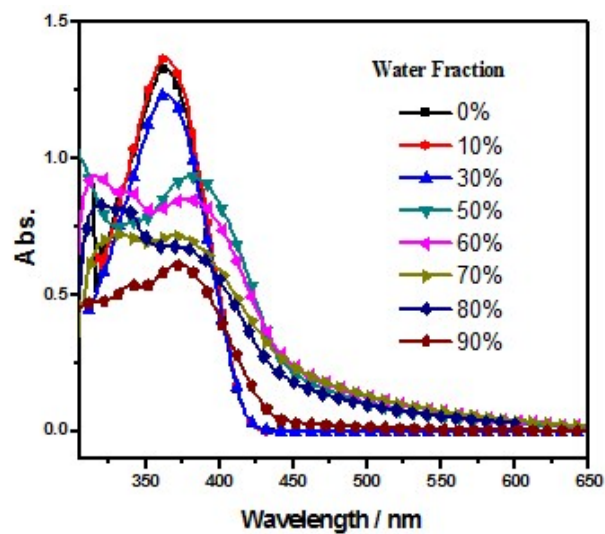
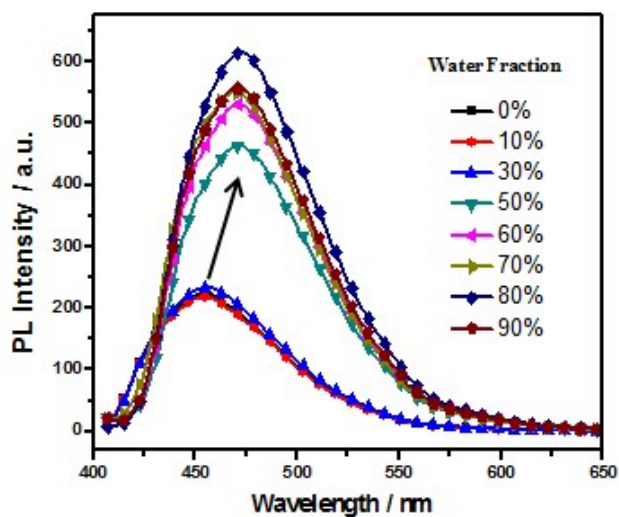


Fig. S5 Crystals of DPCP under sunlight (a) and 365 nm UV irradiation (b).



(a)



(b)

Fig. S6 UV-vis absorption (a) and photoluminescence spectra of DPCP (b) in water/acetone mixtures with different volume fractions of water. Concentration: 0.05 mM.

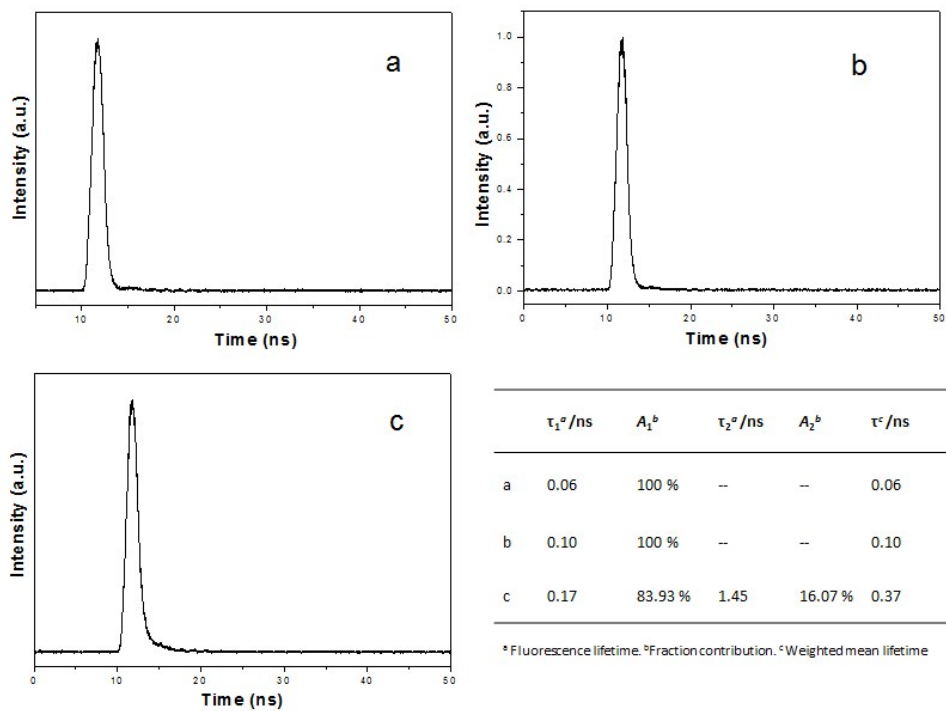


Fig. S7 The fluorescence lifetime curves of DPCP particles in methanol solution (a-b) and methanol/water mixture solution (c).

Table S1. Crystallographic Data and Structure Refinements for **DPCP**

Empirical formula	C ₃₅ H ₂₄ S
Formula weight	476.60
Crystal system	Orthorhombic
Space group	<i>Pca2(1)</i>
<i>a</i> (Å)	13.805(3)
<i>b</i> (Å)	23.501(6)
<i>c</i> (Å)	7.6773(18)
Volume (Å ³)	2490.7(10)
<i>Z</i>	4
D _{Calc} (mg/m ⁻³)	1.271
μ (mm ⁻¹)	0.152
F(000)	1000
<i>R</i> _{int}	0.0513
GOF on <i>F</i> ²	1.026
<i>R</i> ₁ [<i>I</i> >2σ(<i>I</i>)]*	0.0527
<i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)]*	0.1051
<i>R</i> ₁ (all data) *	0.0916
<i>wR</i> ₂ (all data)*	0.1178

Table S2 Selected bond lengths [\AA] and angles [$^\circ$] for **DPCP**.

C(1)-C(2)	1.372(4)	C(28)-C(29)	1.411(4)
C(1)-C(6)	1.461(4)	C(28)-C(30)	1.449(4)
C(1)-C(5)	1.486(4)	C(29)-S(1)	1.747(3)
C(2)-C(3)	1.470(4)	C(30)-C(35)	1.398(4)
C(2)-C(12)	1.491(3)	C(30)-C(31)	1.404(4)
C(3)-C(4)	1.407(3)	C(31)-C(32)	1.357(5)
C(4)-C(5)	1.445(4)	C(32)-C(33)	1.384(5)
C(4)-C(18)	1.469(4)	C(33)-C(34)	1.403(5)
C(6)-C(7)	1.395(4)	C(34)-C(35)	1.375(4)
C(6)-C(11)	1.396(4)	C(35)-S(1)	1.760(3)
C(7)-C(8)	1.380(4)	C(2)-C(1)-C(6)	130.4(3)
C(8)-C(9)	1.354(5)	C(2)-C(1)-C(5)	107.6(3)
C(9)-C(10)	1.375(5)	C(6)-C(1)-C(5)	122.0(2)
C(10)-C(11)	1.383(5)	C(1)-C(2)-C(3)	109.1(2)
C(12)-C(17)	1.384(4)	C(1)-C(2)-C(12)	128.6(3)
C(12)-C(13)	1.394(4)	C(3)-C(2)-C(12)	122.3(2)
C(13)-C(14)	1.367(4)	C(4)-C(3)-C(2)	108.3(3)
C(14)-C(15)	1.374(5)	C(3)-C(4)-C(5)	107.7(3)
C(15)-C(16)	1.372(5)	C(3)-C(4)-C(18)	128.0(3)
C(16)-C(17)	1.387(4)	C(5)-C(4)-C(18)	124.3(2)
C(18)-C(23)	1.380(4)	C(4)-C(5)-C(1)	107.3(2)
C(18)-C(19)	1.401(4)	C(7)-C(6)-C(11)	116.9(3)
C(19)-C(20)	1.370(4)	C(7)-C(6)-C(1)	120.8(3)
C(20)-C(21)	1.393(4)	C(11)-C(6)-C(1)	122.3(3)
C(21)-C(22)	1.389(4)	C(8)-C(7)-C(6)	121.3(3)
C(21)-C(24)	1.485(4)	C(9)-C(8)-C(7)	121.0(3)

C(22)-C(23)	1.378(4)	C(8)-C(9)-C(10)	119.1(3)
C(24)-C(25)	1.392(4)	C(9)-C(10)-C(11)	120.9(3)
C(24)-C(29)	1.400(4)	C(10)-C(11)-C(6)	120.7(3)
C(25)-C(26)	1.389(5)	C(17)-C(12)-C(13)	117.8(3)
C(26)-C(27)	1.365(4)	C(17)-C(12)-C(2)	122.0(3)
C(27)-C(28)	1.386(5)	C(13)-C(12)-C(2)	120.1(3)
C(14)-C(13)-C(12)	121.0(3)	C(27)-C(26)-C(25)	120.8(4)
C(13)-C(14)-C(15)	120.8(3)	C(26)-C(27)-C(28)	119.4(3)
C(16)-C(15)-C(14)	119.2(3)	C(27)-C(28)-C(29)	120.2(3)
C(15)-C(16)-C(17)	120.5(3)	C(27)-C(28)-C(30)	128.5(3)
C(12)-C(17)-C(16)	120.7(3)	C(29)-C(28)-C(30)	111.4(3)
C(23)-C(18)-C(19)	116.4(3)	C(24)-C(29)-C(28)	120.7(3)
C(23)-C(18)-C(4)	120.4(3)	C(24)-C(29)-S(1)	126.8(2)
C(19)-C(18)-C(4)	123.1(2)	C(28)-C(29)-S(1)	112.5(2)
C(20)-C(19)-C(18)	121.7(3)	C(35)-C(30)-C(31)	118.3(3)
C(19)-C(20)-C(21)	121.8(3)	C(35)-C(30)-C(28)	112.9(3)
C(22)-C(21)-C(20)	116.2(3)	C(31)-C(30)-C(28)	128.6(3)
C(22)-C(21)-C(24)	122.1(2)	C(32)-C(31)-C(30)	119.4(4)
C(20)-C(21)-C(24)	121.6(3)	C(31)-C(32)-C(33)	121.8(3)
C(23)-C(22)-C(21)	121.9(3)	C(32)-C(33)-C(34)	120.4(3)
C(22)-C(23)-C(18)	121.8(3)	C(35)-C(34)-C(33)	117.3(4)
C(25)-C(24)-C(29)	117.2(3)	C(34)-C(35)-C(30)	122.7(3)
C(25)-C(24)-C(21)	118.8(3)	C(34)-C(35)-S(1)	125.5(3)
C(29)-C(24)-C(21)	124.1(3)	C(30)-C(35)-S(1)	111.7(2)
C(26)-C(25)-C(24)	121.8(3)	C(29)-S(1)-C(35)	91.37(15)