Electronic Supplementary Information

Self-assembly of sodium 4-(4,5-diphenyl-1H-imidazol-2-yl)benzoate into ultralong microbelts

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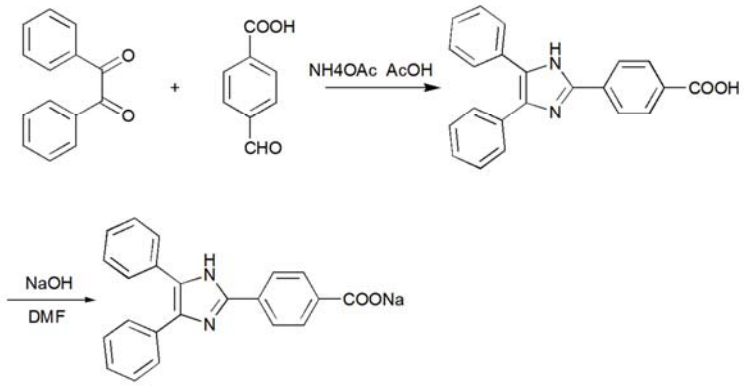
S1. Synthesis of sodium 4-(4,5-diphenyl-1H-imidazol-2-yl)benzoate (SDB)



Synthesis of 4-(4,5-diphenyl-1H-imidazol-2-yl)benzyl acid (DBA): Benzil (2.10 g, 10.0 mmol), (4-formylbenzyl acid) (1.50 g, 10.0 mmol), and ammonium acetate (7.70 g, 0.100 mol) were dissolved in glacial acetic acid (50 mL) and then refluxed for 6 h. The reaction was monitored by thin layer chromatography. After cooling to room temperature, the reaction mixture was poured into cool water and collected on a filter. The solid was washed with cool water and purified by silica gel chromatography using ethyl acetate/petroleum ether (1:1, v/v) as an eluent to isolate pure DBA. (2.65 g, 75%). ^{1}H NMR (400 MHz, DMSO-d$_6$) δ (ppm): 12.97 (s, 1H, COOH), 12.90 (s, 1H, NH), 8.18 (d, 2H, ArH), 8.01 (d, 2H, ArH), 7.54-7.22 (m, 10H, ArH). MS ($C_{22}H_{16}N_2O_2$) m/z: calcd for 340.12, found: 341.12 $[M + H]^+$.

Synthesis of SDB: To the solution of DBA (0.34 g, 1.0 mmol) in DMF (30 mL), aqueous solution of sodium hydroxide (2.0 g, 50 mmol, in 10 mL water) was added dropwise. The reaction mixture was stirred at 150 °C for 3 h. After cooling to room temperature, the solution was poured into ice-water. The solid was filtered off and washed with water (3 × 100 mL), and then dried in *vacuo* (223 mg, 63 %). ^{1}H NMR (400 MHz, DMSO-d$_6$) δ (ppm): 12.90 (s, 1H, NH), 8.18 (d, 2H, ArH), 8.01 (d, 2H, ArH), 7.54-7.31 (m, 10H, ArH).

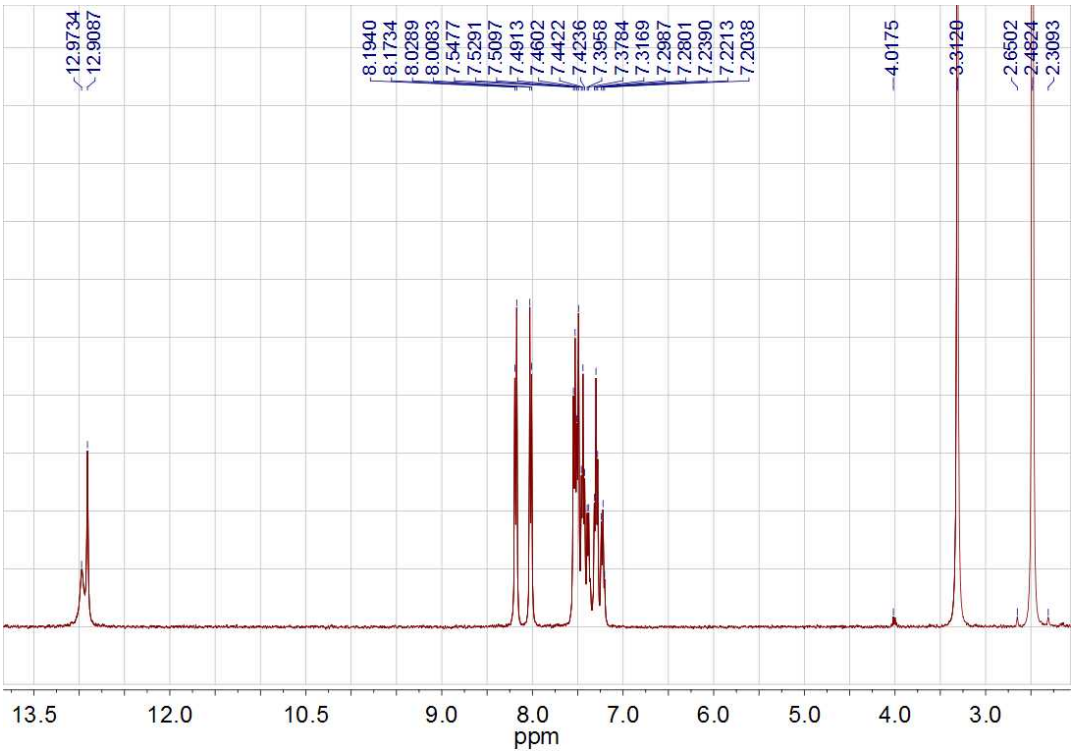


Fig. S1. ^{1}H NMR spectrum of DBA in DMSO-d_6.

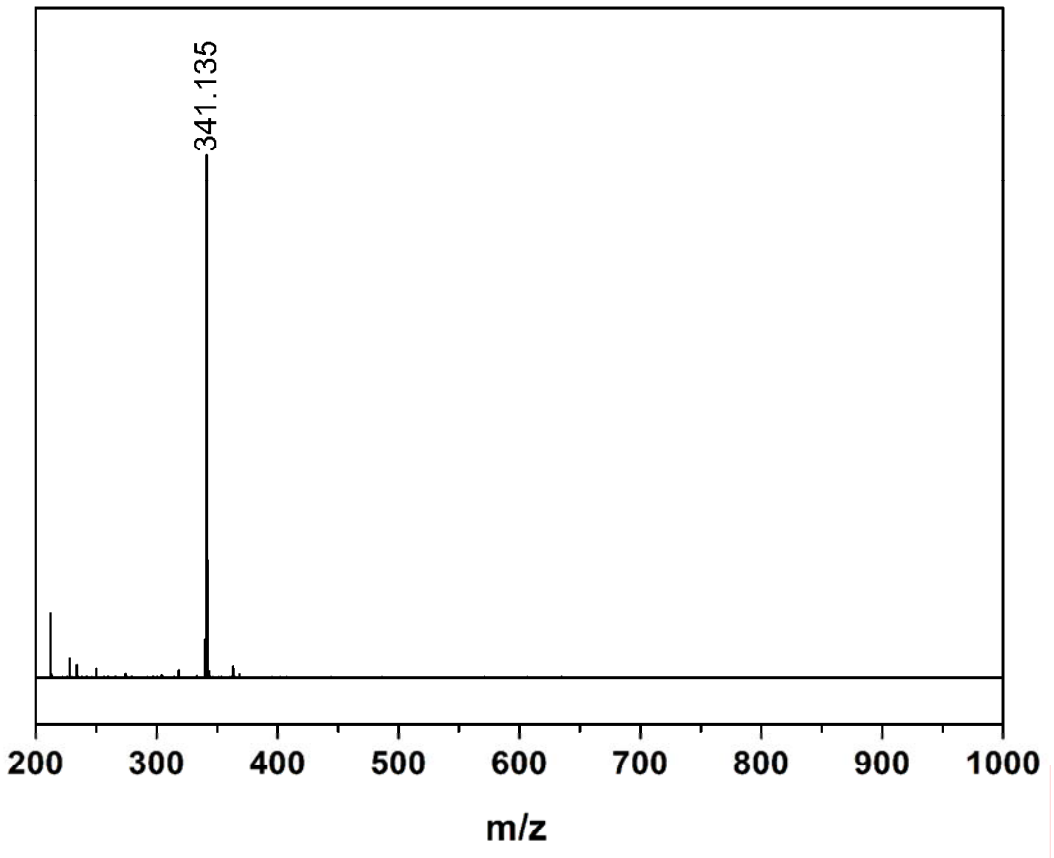


Fig. S2. MS spectrum of DBA.

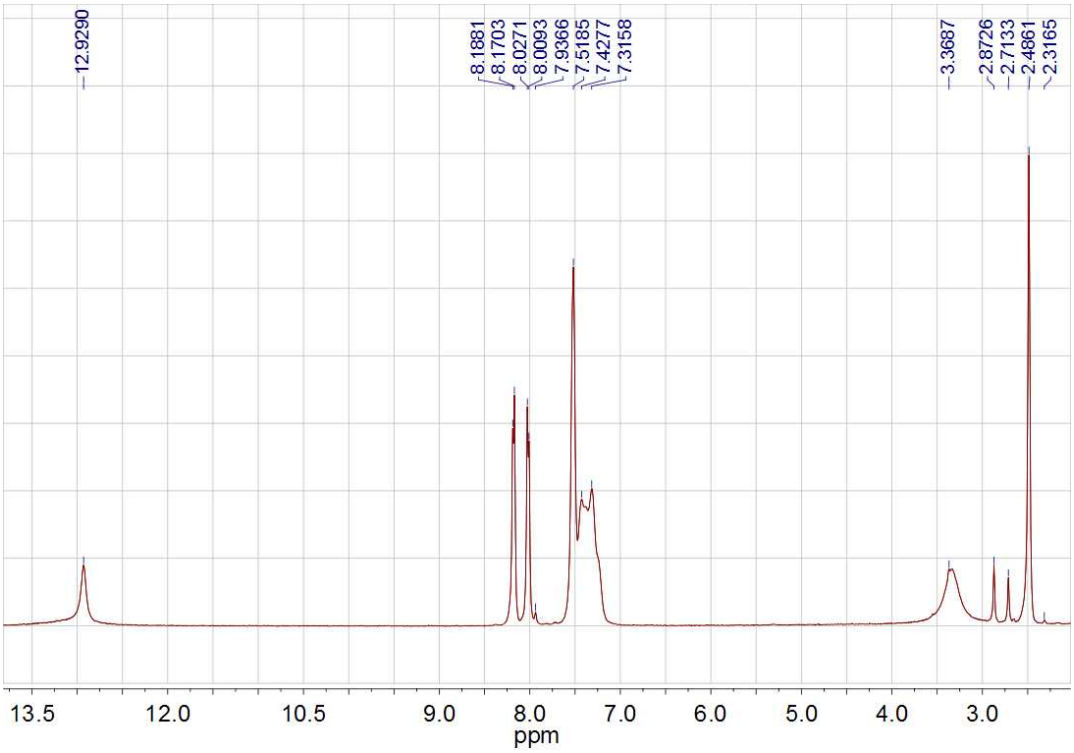


Fig. S3. ^{1}H NMR spectrum of SDB in DMSO-d_6.

S2. The X-ray powder diffraction patterns of the SDB raw powder and SDB microbelts are indexed with program Powder-X

Table S1. Indexing results of the SDB raw powder diffraction pattern were shown below.

The crystal structure is monoclinic, a = 8.617088 Å, b = 12.32580 Å, c = 6.402258 Å, Alpha = 90.00000°, Beta = 111.3478°, Gama = 90.00000°, Volume =637.3581 Å^3.

h	k	l	2Theta (Exp.)	2Theta (Calc.)	2Theta (Diff.)	*d* (Exp.)	*d* (Calc.)
0	1	0	7.166	7.166	0.000	12.3254	12.3258
-1	0	0	11.065	11.015	0.050	7.98984	8.02585
-1	1	0	13.132	13.153	-0.021	6.73641	6.72571

0	2	0	14.194	14.36	-0.166	6.23469	6.1629
0	0	1	14.798	14.844	-0.047	5.98171	5.96298
0	1	1	16.527	16.501	0.026	5.35952	5.36782
-1	2	0	18.134	18.134	0.000	4.88805	4.88805
0	2	1	20.684	20.71	-0.026	4.29074	4.2854
1	0	1	21.478	21.542	-0.064	4.13392	4.12179
-2	0	0	21.954	22.134	-0.179	4.0453	4.01292
-2	1	1	22.885	22.894	-0.008	3.8828	3.88139
-1	3	0	24.354	24.318	0.036	3.65195	3.65724
1	2	1	25.994	25.986	0.009	3.42503	3.42615
-1	0	2	27.86	27.849	0.011	3.19979	3.20103
0	0	2	29.831	29.946	-0.114	2.99265	2.98149
1	3	1	30.538	30.701	-0.162	2.92497	2.90987
-2	3	0	31.127	31.129	-0.002	2.87096	2.87079
-1	4	1	32.864	32.725	0.139	2.72312	2.73434
0	2	2	33.249	33.358	-0.109	2.69245	2.68391
-1	3	2	35.104	35.523	-0.419	2.55431	2.52511

Table S2. Indexing results of the SDB microbelts diffraction pattern were shown below.

The crystal structure is monoclinic, a = 17.06874 Å, b = 4.348648 Å, c = 14.14148 Å, Alpha = 90.00000°, Beta = 112.8837°, Gama = 90.00000°, Volume =967.0519 Å^3.

h	k	l	Theta (Exp.)	Theta (Calc.)	Theta (Diff.)	*d* (Exp.)	*d* (Calc.)
0	0	1	6.649	6.651	-0.002	13.28403	13.27972
-2	0	1	10.604	10.607	-0.003	8.33617	8.33403
-2	0	0	11.244	11.244	-0.001	7.86322	7.86268
0	0	2	13.356	13.324	0.032	6.62403	6.63986
2	0	1	14.736	15.152	-0.416	6.00666	5.84261
2	0	1	15.296	15.152	0.144	5.78798	5.84261
-3	0	1	15.496	15.562	-0.066	5.71373	5.68946
1	0	2	16.366	16.373	-0.008	5.4119	5.40941
-3	0	0	16.906	16.901	0.005	5.24023	5.24179
-3	0	2	17.436	16.979	0.456	5.08212	5.21771
0	0	3	19.621	20.043	-0.422	4.52082	4.42657
1	1	0	21.133	21.18	-0.047	4.20063	4.19134
-1	1	1	21.52	21.544	-0.023	4.1259	4.12147
-4	0	0	22.589	22.599	-0.010	3.93313	3.93134
-1	1	2	23.816	23.884	-0.068	3.73315	3.72271
0	1	2	24.428	24.449	-0.021	3.64097	3.63788

-5	0	2	26.126	26.194	-0.068	3.40808	3.39938
0	0	4	26.844	26.832	0.012	3.31846	3.31993
-5	0	3	27.669	27.655	0.014	3.22139	3.22298
0	1	3	28.846	28.755	0.091	3.0926	3.10214
-3	1	3	29.184	29.159	0.025	3.05749	3.06007
-4	1	2	29.616	29.669	-0.053	3.01393	3.00869
-3	0	5	31.253	31.255	-0.001	2.85965	2.85954
-1	0	5	31.864	31.89	-0.025	2.80619	2.80402
-6	0	1	32.123	32.11	0.012	2.78423	2.78526
-3	1	4	32.896	32.921	-0.025	2.72052	2.71851
0	0	5	33.729	33.719	0.010	2.65518	2.65594

S3. The possible packing structure of SDB molecules

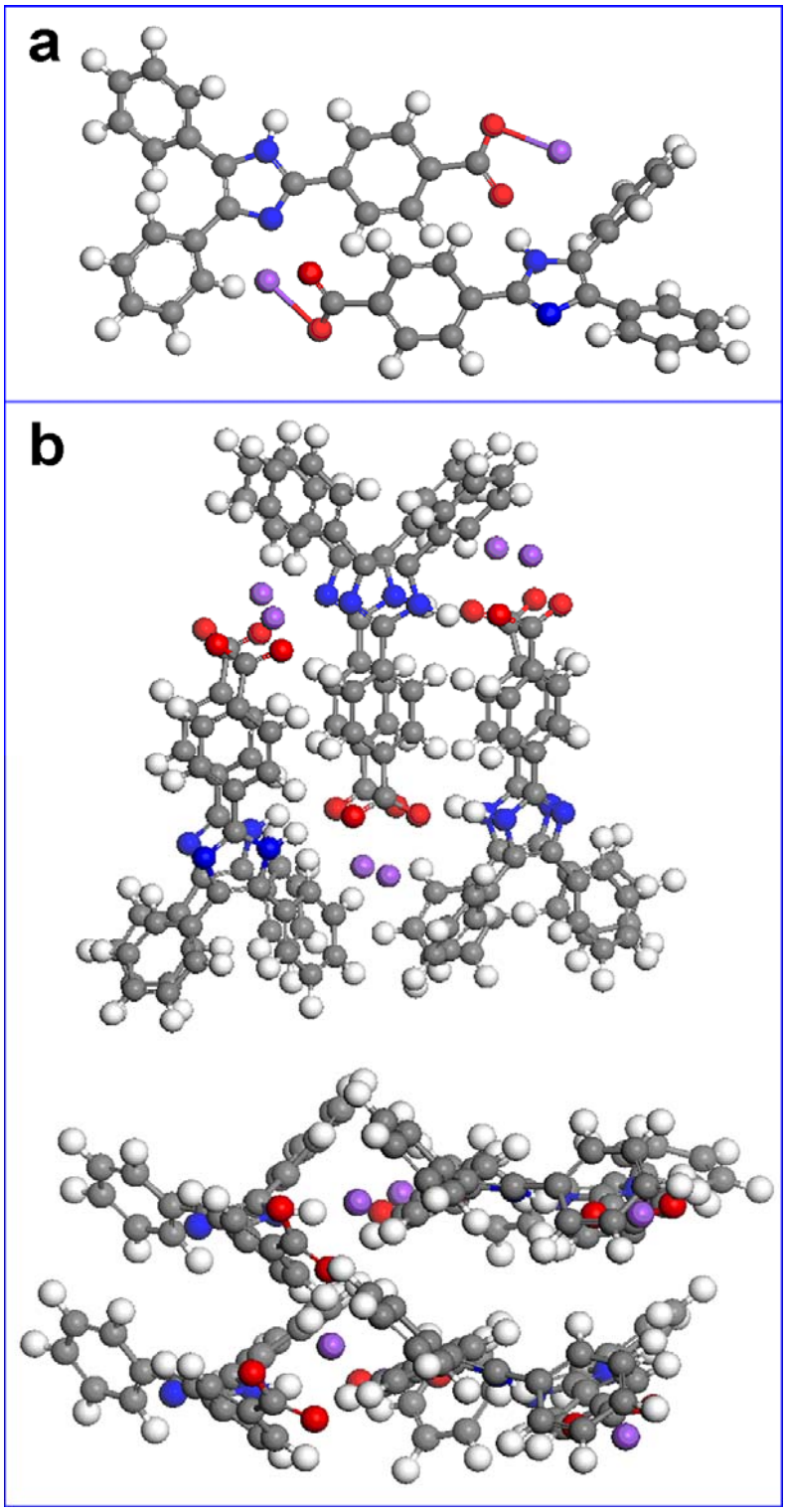


Fig. S4. (a) Optimized packing structure of SDB molecular dimer. (b) Side view and top view of the optimized hexamer structure of SDB molecules.

S4. The optical properties of the as-prepared SDB microbelts as well as the SDB raw powder

For the UV-vis and fluorescence measurements, the SDB raw powder was dissolved in THF and diluted to suitable concentration. Similarly, SDB raw powder was dispersed in water and diluted to suitable concentration. Before test, it is necessary to shake the cuvette to prevent the precipitation of SDB powder. Considering the fact that the microbelts are easily broken, the as-prepared SDB microbelts suspended in water were not separated, but were directly diluted with water to obtain a suitable concentration for optical measurements. Again, it is necessary to shake the cuvette gently to prevent the precipitation of SDB microbelts before each test. For the solid state UV-vis and fluorescence measurements, the sample was prepared by spin coating SDB solution in THF or SDB microbelts suspension in water onto clear quartz slide at 2000 rpm.

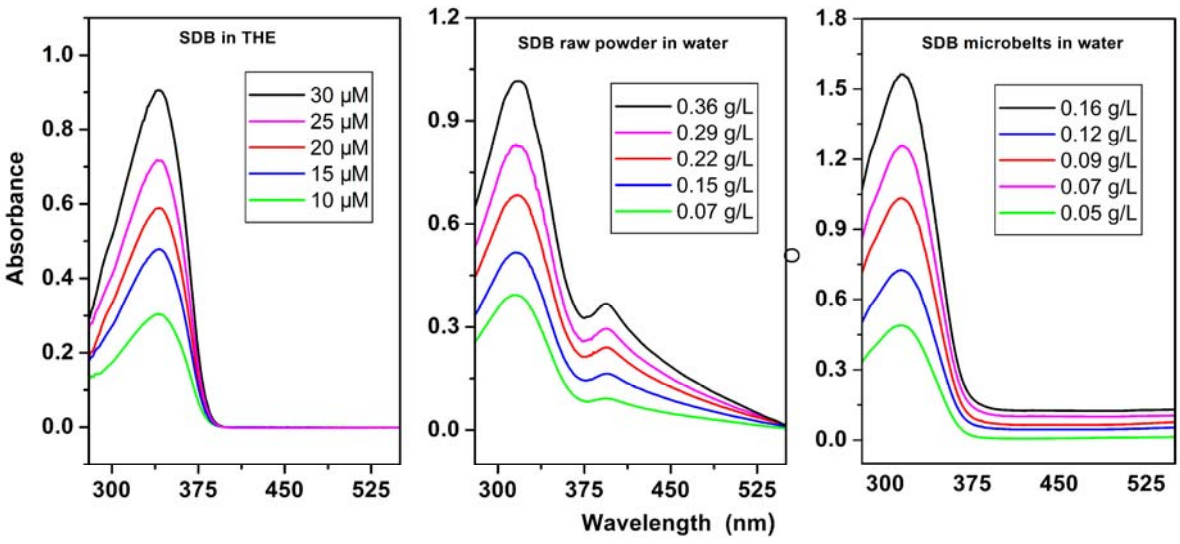


Fig. S5. Concentration dependent UV-vis spectra of SDB solution in THF, SDB raw powder dispersed in water, and SDB microbelts (with length of about 5 mm) dispersed in water.

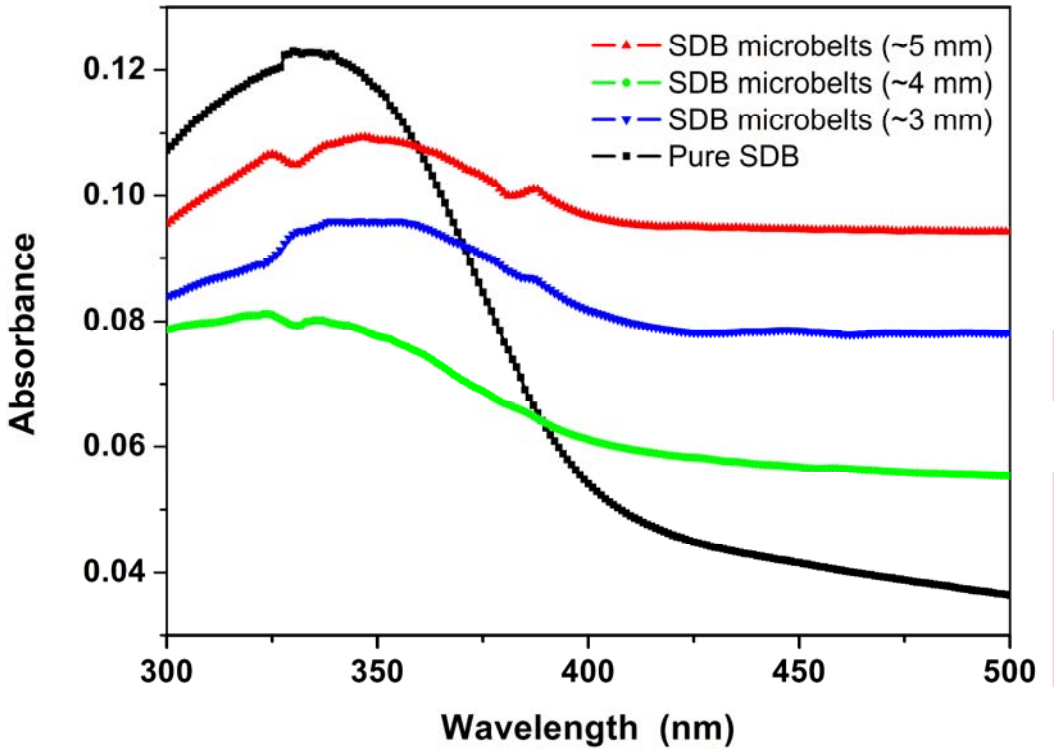


Fig. S6. Solid state UV-vis spectra of SDB monomer and SDB microbelts. The sample was prepared by spin coating SDB solution in THF or SDB microbelts suspension in water onto clear quartz slide.

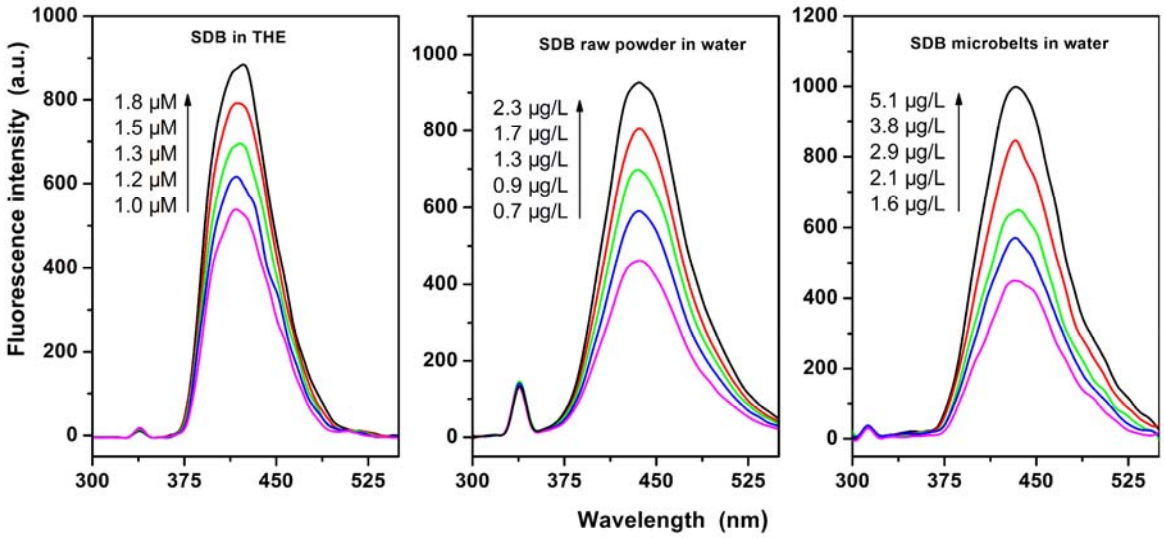


Fig. S7. Concentration dependent fluorescence spectra of SDB solution in THF, SDB raw powder dispersed in water, and SDB microbelts (with length of about 5 mm) dispersed in water.

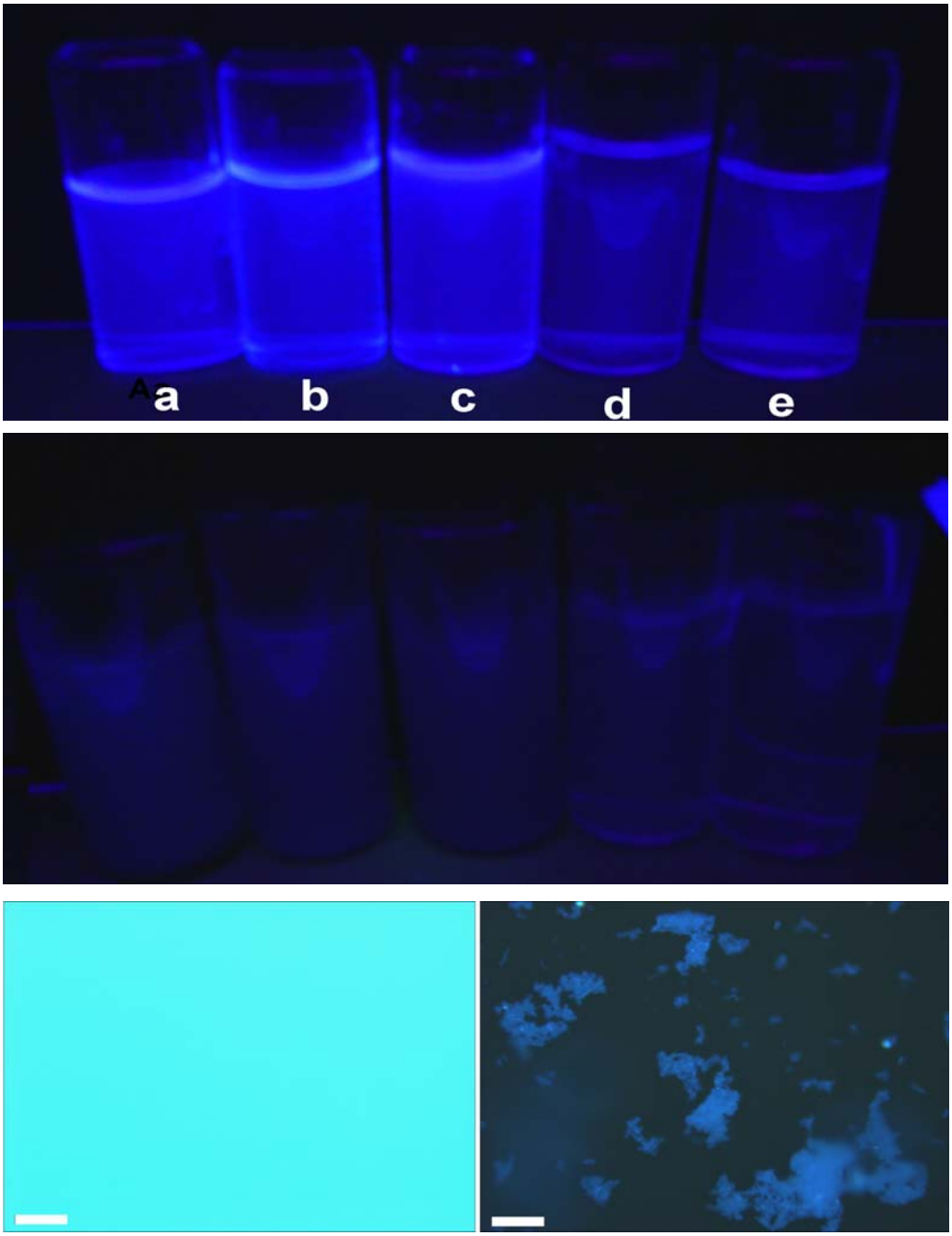


Fig. S8. Concentration dependent fluorescence images under a UV lamp at 365 nm. (Top) SDB solution in THF (30 mM, 10 mM, 0.5 mM, 5 μM, 0.05 μM), (Middle) SDB raw powder dispersed in water. (Bottom) Fluorescence images obtained by MF30 fluorescence microscope. SDB solution in THF (left), SDB raw powder dispersed in water (right), a droplet of solution or suspension was placed onto glass substrate and then subjected to observation immediately. Scale bar = 500 μm.

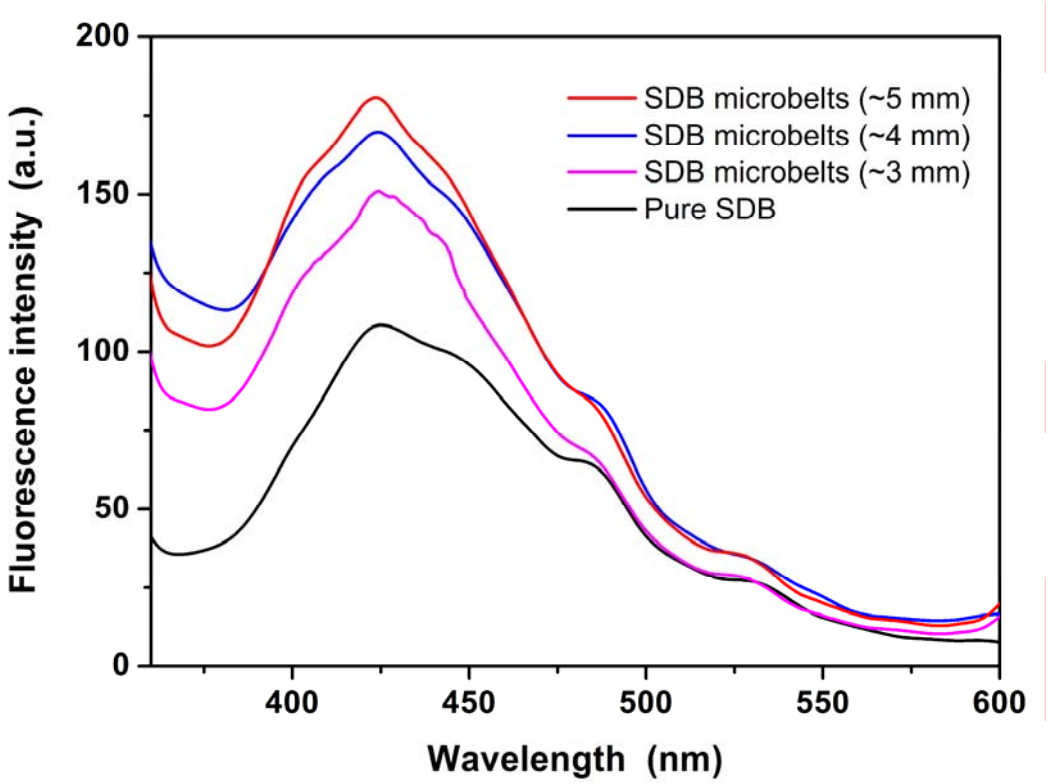


Fig. S9. Solid state fluorescence spectra of SDB monomer and SDB microbelts. The sample was prepared by spin coating SDB solution in THF or SDB microbelts suspension in water onto clear quartz slide.

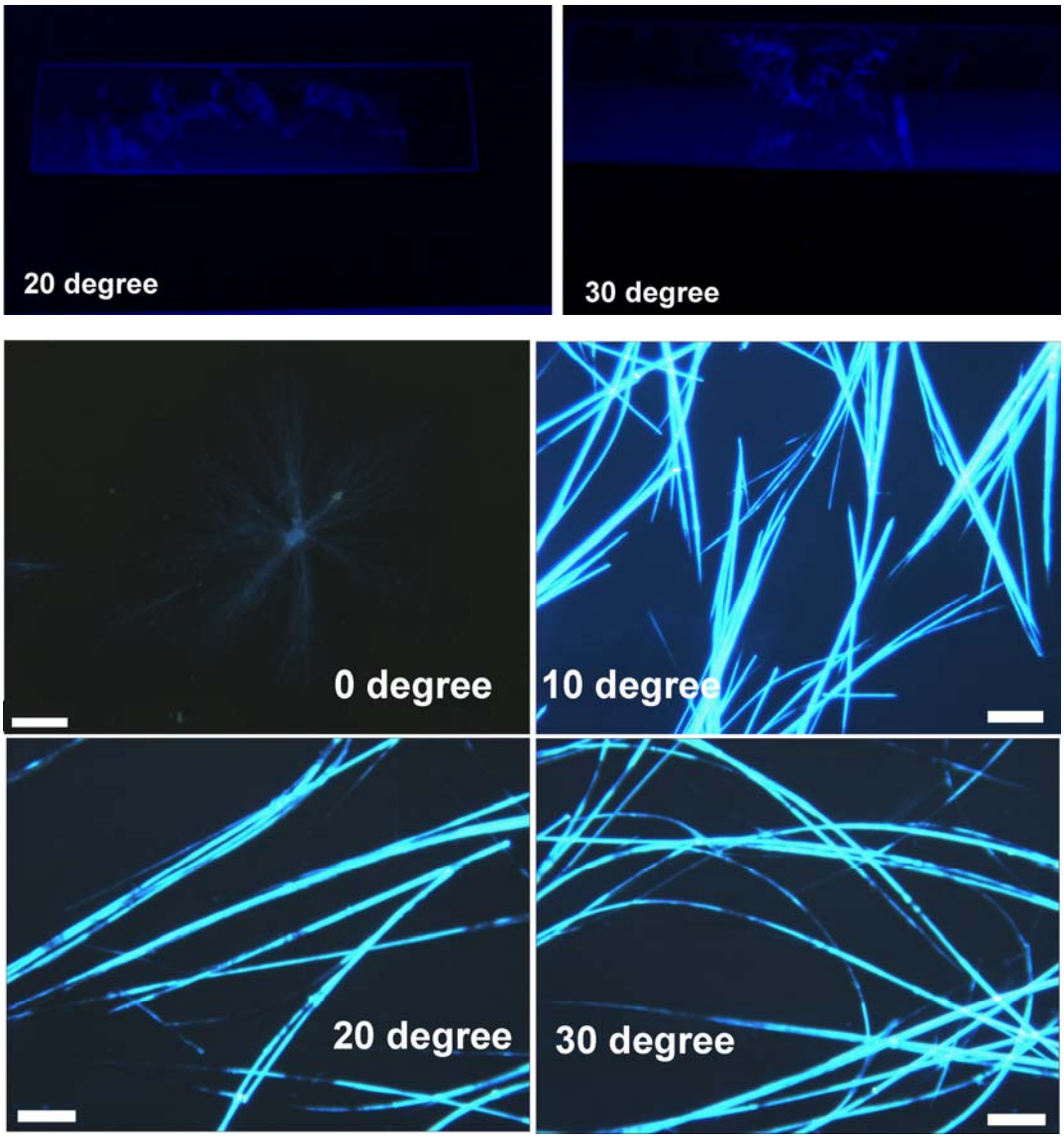


Fig. S10. Solid state UV-Vis patterns (top) and fluorescence images (bottom) of self-assembled SDB prepared at different temperature. Scale bar = 500 μm.

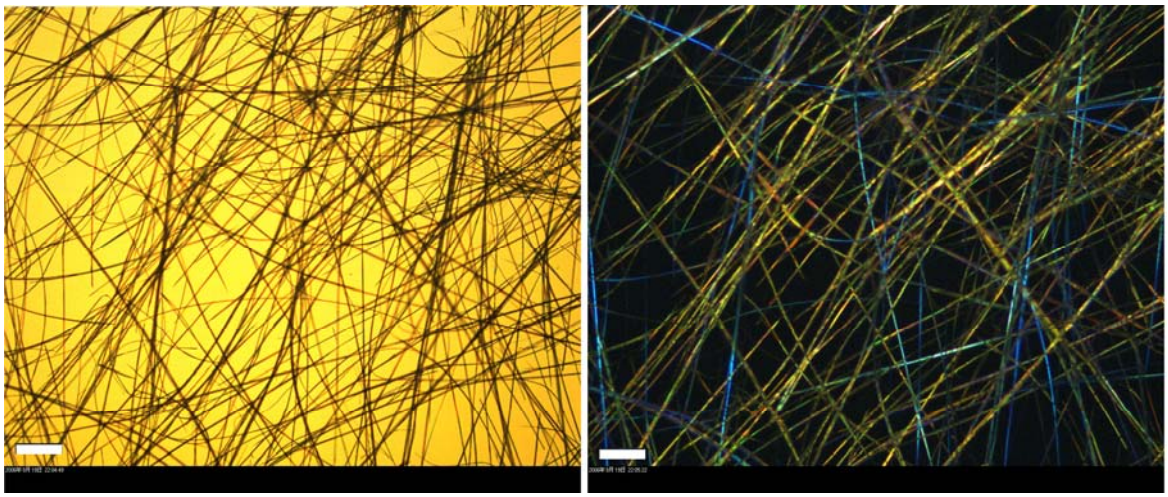


Fig. S11. Optical microscope (left) and polarized optical microscope (right) imagines of SDB microbelts prepared at SDB concentration of 3 mM. The apparent length of microbelts reaches several millimeter and endless fibers were detected under the visual field.

Fig. S12. The digital photographs of the as-prepared microbelts .