## **Supplementary Materials**

DHTPz-Bt COF: Space group symmetry P3													
a = b = 30.02  Å, c = 3.81  Å													
$alpha = beta = 90^{\circ}, gamma = 120^{\circ}$													
Atom	x (Å)	y (Å)	z (Å)	Atom	x (Å)	y (Å)	z (Å)						
C1	0.34732	-0.28056	-0.00251	O50	0.50578	-0.11417	-0.04617						
C2	0.29717	-0.31632	-0.0789	O51	0.88251	-0.61352	0.0414						
C3	0.28309	-0.36639	-0.10154	O52	0.49998	-0.88445	0.01693						
C4	0.31974	-0.38045	-0.05686	C53	0.53676	-0.01584	-0.10204						
C5	0.36965	-0.34497	0.03563	C54	0.4539	-0.03471	0.09618						
C6	0.3826	-0.29538	0.07989	C55	0.47187	-0.9835	0.11342						
C7	0.23079	-0.40628	-0.16012	C56	0.55655	-0.96468	-0.05804						
C8	0.40868	-0.35907	0.05917	C57	0.98331	-0.54828	0.06263						
N9	0.40179	-0.40109	-0.05671	C58	0.96662	-0.47994	0.09877						
N10	0.44128	-0.4123	-0.04098	C59	0.01808	-0.44835	0.1076						
C11	0.42854	-0.45935	0.08223	C60	0.03447	-0.51673	0.10415						
C12	0.46444	-0.47776	0.07357	O61	0.45446	-0.60126	-0.10142						
O13	0.38483	-0.48838	0.18586	O62	0.53801	-0.40442	0.34986						
C14	0.44595	-0.52771	-0.02737	O63	0.60763	-0.93545	-0.14445						
C15	0.47629	-0.54998	-0.04206	O64	0.93294	-0.46316	0.17034						
C16	0.52963	-0.51878	0.00532	O65	0.0646	-0.53779	0.16711						
C17	0.54758	-0.46815	0.09118	O66	0.4075	-0.06909	0.24348						
C18	0.5162	-0.44902	0.15879	H67	0.26908	-0.30521	-0.12945						
C19	0.56754	-0.53513	-0.02595	H68	0.31049	-0.41932	-0.08943						
N20	0.55619	-0.584	0.01121	H69	0.42104	-0.26636	0.15894						
N21	0.59572	-0.59516	-0.00899	H70	0.2238	-0.44283	-0.23317						
C22	0.58661	-0.64034	-0.01764	H71	0.44667	-0.3312	0.13748						
O23	0.61182	-0.50322	-0.07602	H72	0.47585	-0.38983	-0.18421						
C24	0.6277	-0.65201	-0.03259	H73	0.40535	-0.54911	-0.08626						
C25	0.61538	-0.70173	-0.02373	H74	0.58763	-0.44214	0.13138						
C26	0.65334	-0.71429	-0.02907	H75	0.51756	-0.61201	0.05412						
C27	0.70411	-0.67648	-0.05016	H76	0.54728	-0.67102	-0.01271						
C28	0.71685	-0.62672	-0.07156	H77	0.57621	-0.7317	-0.01031						
C29	0.67834	-0.61452	-0.05945	H78	0.73478	-0.68521	-0.04975						
C30	0.76982	-0.58625	-0.09006	H79	0.68741	-0.57576	-0.06817						
N31	0.80681	-0.59564	-0.0803	H80	0.77816	-0.54771	-0.09428						
C32	0.64113	-0.7666	-0.01392	H81	0.67181	-0.7748	-0.01612						
N33	0.59469	-0.80385	-0.01047	H82	0.33448	-0.21623	0.03197						
N34	0.19339	-0.39928	-0.08255	H83	0.43875	-0.20355	-0.15805						
C35	0.36234	-0.22786	-0.01805	H84	0.39481	-0.12843	-0.12761						
C36	0.40946	-0.19235	-0.10058	H85	0.12805	-0.47228	-0.19662						

 Table S1. Fractional atomic coordinates for DHTPz-Bt COF unit cell.

N37	0.42255	-0.14038	-0.10072	H86	0.87075	-0.51944	-0.13473
N38	0.14199	-0.43743	-0.08146	H87	0.61342	-0.86248	0.03431
N39	0.85817	-0.55774	-0.07863	H88	0.56269	-0.02805	-0.1824
N40	0.58441	-0.8542	-0.01069	H89	0.44489	-0.97087	0.18203
C41	0.53496	-0.8935	0.00749	H90	0.97172	-0.58746	0.04847
C42	0.52237	-0.94713	0.02953	H91	0.03296	-0.4078	0.11823
C43	0.89446	-0.56988	0.00669	H92	0.41567	-0.62121	-0.0904
C44	0.94819	-0.53177	0.0538	H93	0.51269	-0.39078	0.40357
C45	0.10762	-0.42822	0.08607	H94	0.63022	-0.91411	0.05605
C46	0.05291	-0.46534	0.10239	H95	0.94943	-0.42494	0.20278
C47	0.47242	-0.10364	-0.05595	H96	0.10318	-0.5131	0.21257
C48	0.48687	-0.0508	-0.0249	H97	0.38487	-0.05437	0.3183
O49	0.12296	-0.38856	0.23542				



**Fig. S1.** The simulated AA stacking eclipse model for DHTPz-Bt showing (a) one quarter of a frame unit and (b) a whole frame unit.



**Fig. S2.** The FTIR spectra obtained from DHTPz, Bt, DHTPz-Bt and DHTPz-Bt@Zn<sup>2+</sup>. The peaks related to various functional groups are labeled.



Fig. S3. The SEM image of the DHTPz-Bt.



Fig. S4. The thermogravimetric curve of the DHTPz-Bt.



Fig. S5. The fluorescence spectra of DHTPz-Bt in different dispersion solvents (a) before and (b) after the addition of  $Zn^{2+}$ .  $E_x = 395$  nm; DHTPz-Bt concentration: 20 mg/L;  $Zn^{2+}$  concentration: 45  $\mu$ mol/L.



Fig. S6. Fluorescence intensities of DHTPz-Bt before and after the addition of  $Zn^{2+}$  in different solvents. DHTPz-Bt concentration: 20 mg/L;  $Zn^{2+}$  concentration: 45 µmol/L;  $E_x = 395$  nm;  $E_m = 513$  nm.



Fig. S7. The XPS spectra of the DHTPz-Bt and DHTPz-Bt@Zn<sup>2+</sup> complex.