Supporting Information for

BODIPY and *N*-halamine decorated covalent organic framework with synergistic antibacterial capabilities for sunlight-powered water sterilization

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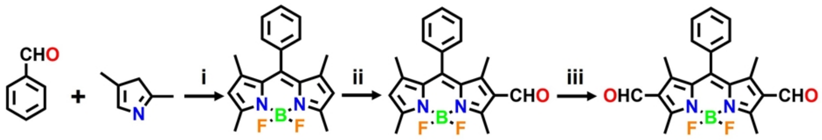
1. Synthesis and characterization of BDP[1]



intermediate A   Intermediate B   BDP

Fig. S1 Synthesis of **BDP**. (i). 1) DCM, TFA; 2) TCBQ; 3) TEA, $BF_3 \cdot OEt_2$; (ii). $POCl_3$, DMF, DCE; (iii). $POCl_3$, DMF, DCE

Synthesis of intermediate A. Mixture of benzaldehyde (510 µL, 5.0 mmol), 2,4-dimethylpyrrole (1.28 mL, 12.5 mmol), and TFA (70 µL, 1.0 mmol) in dry DCM (20 mL) was reacted for 3 h at 25 °C. Subsequently, tetrachlorobenzoquinone (TCBQ) was added to the reaction mixture and reacted for 1 h. After that, triethylamine (TEA) (4 mL) and $BF_3 \cdot OEt_2$ (5 mL) were added slowly and stirred for another 1 h at 25 °C. After quenching the reaction with H_2O and removal of the solvent in vacuum, the crude product was purified via column chromatography (eluent: EtOAc: PE, 1/100, *v*/*v*) to afford **intermediate A** (128 mg) as an orange-red crystalline solid in 79 % yield.

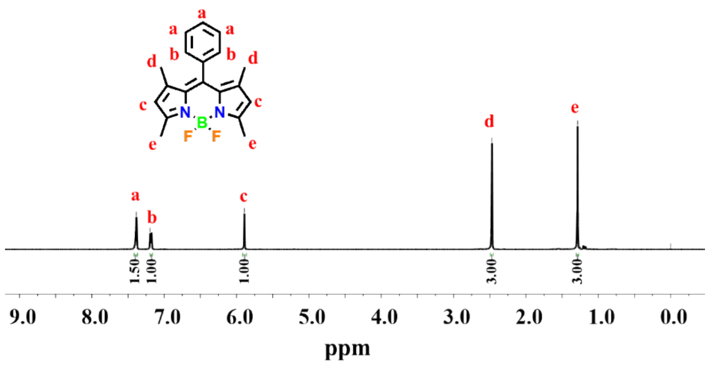


Fig. S2 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **intermediate A**, δ (ppm): 7.40~7.38 (t, 3H), 7.19 (d, 2H), 5.89 (s, 2H), 2.47 (s, 6H), 1.28 (s, 6H).

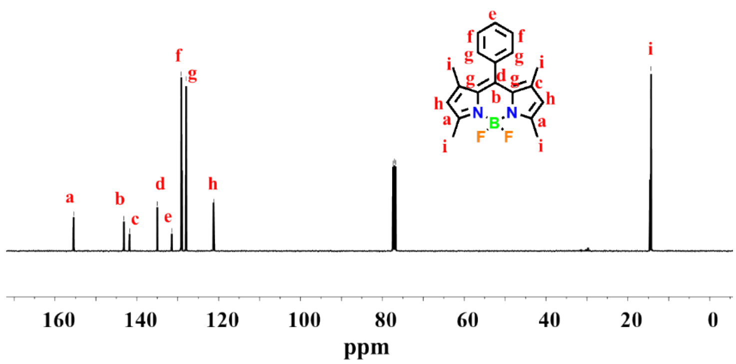


Fig. S3 ^{13}C NMR spectrum(100 MHz, $CDCl_3$) of **intermediate A**, δ (ppm): 155.44, 143.18, 141.77, 129.15, 127.96, 121.22, 14.59, 14.34.

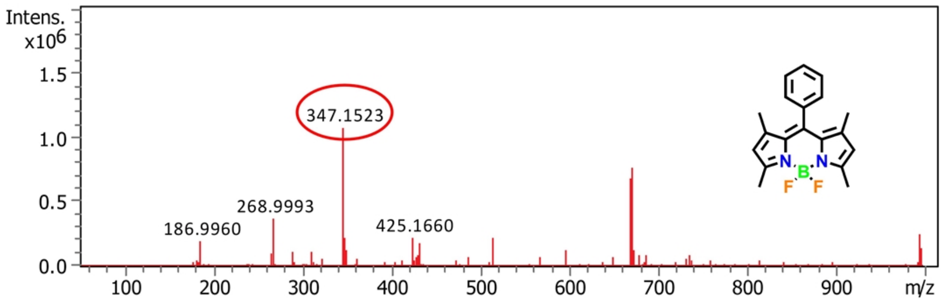


Fig.S4 Mass spectrum (ESI) of **intermediate A**. *m/z* calcd for $[C_{19}H_{19}BF_2N_2+Na]^+$ 347.1502, found, 347.1523.

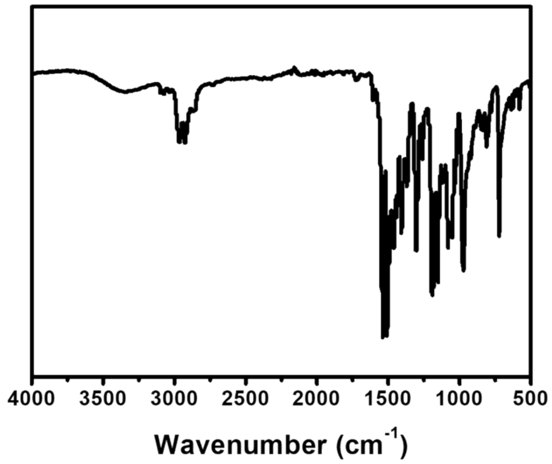


Fig. S5 FTIR spectrum of **intermediate A** (KBr, cm^{-1}): 2963 (w), 2924 (w), 1538 (s), 1507 (s), 1465 (m), 1408 (m), 1369 (w), 1305 (m), 1191 (s), 1154 (s), 1081 (m), 1055 (m), 973 (s), 811 (w), 722 (m).

Synthesis of intermediate B. Intermediate A (150 mg, 0.42 mmol) in dichloroethane (DCE) (20 mL) was added into the DMF (6 mL) solution of $POCl_3$ (6 mL), and the mixture was stirred for 6 h at 25 °C. The reaction was then quenched with saturated $NaHCO_3$ solution (200 mL) in an ice bath. After sequential extraction and column chromatography (eluent: hexane/EtOAc/CH_2Cl_2, 4/1/1, *v*/*v*), **intermediate B** (120 mg) was obtained as a red crystalline solid in 75 % yield.

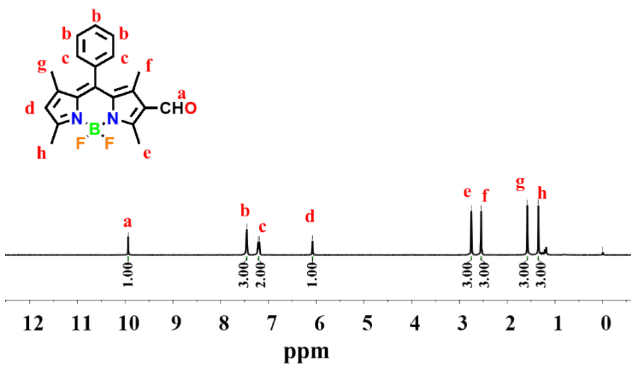


Fig. S6 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **intermediate B**, δ (ppm): 9.93 (s, 1H), 7.45 (t, 3H), 7.19 (d, 2H), 6.08 (s, 1H), 2.75 (s, 3H), 2.55 (s, 3H), 1.58 (s, 3H), 1.35 (s, 3H).

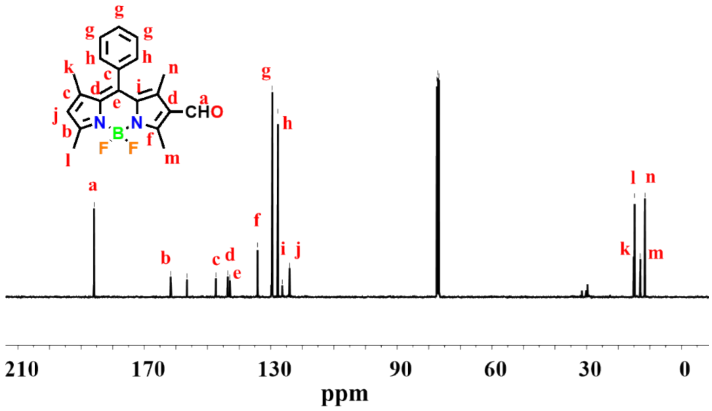


Fig. S7 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **intermediate B**, δ (ppm): 185.91, 161.65, 156.49, 142.92, 134.17, 129.80, 129.50, 127.71, 126.33, 124.02, 15.08, 14.84, 13.02, 11.55.

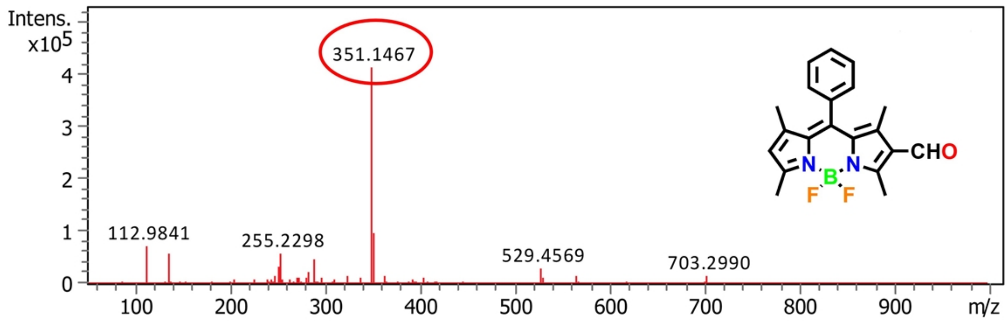


Fig. S8 Mass spectrum (ESI) of **intermediate B**. *m*/*z* calcd for $[C_{20}H_{19}BF_2N_2O\text{-}H]^-$ 351.1551, found, 351.1467.

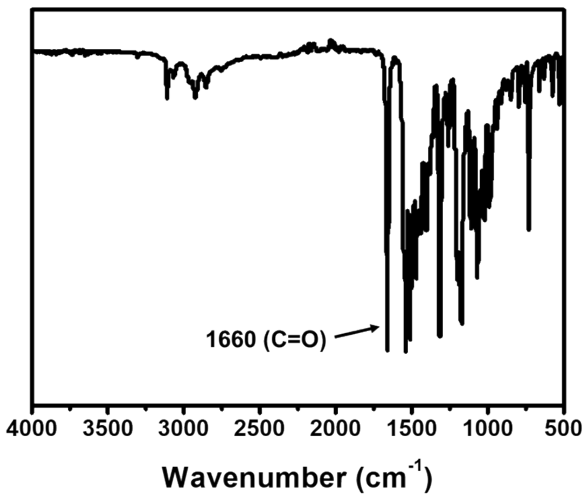


Fig.S9 FTIR spectrum of **intermediate B** (KBr, cm^{-1}): 3110 (w), 2925 (w), 2852 (w), 1660 (s), 1539 (s), 1512 (s), 1472 (m), 1405 (m), 1315 (s), 1259 (w), 1174 (s), 1113 (m), 1068 (m), 1024 (m), 797 (w), 731 (m), 529 (w).

Synthesis of BDP. A mixture of DMF (6 mL) and $POCl_3$ (6 mL) was stirred, **intermediate B** (160 mg, 0.42 mmol) in dichloroethane (DCE) (15 mL) was added, and the mixture was stirred for 12 h. After quenching the reaction with saturated $NaHCO_3$ solution (200 mL) in an ice bath, the crude product was further purified by extraction and column chromatography (eluent: PE: EtOAc, 5/1, *v*/*v,* followed by pure EtOAc) to afford **BDP** (86 mg) as a reddish-brown powder in 51% yield.

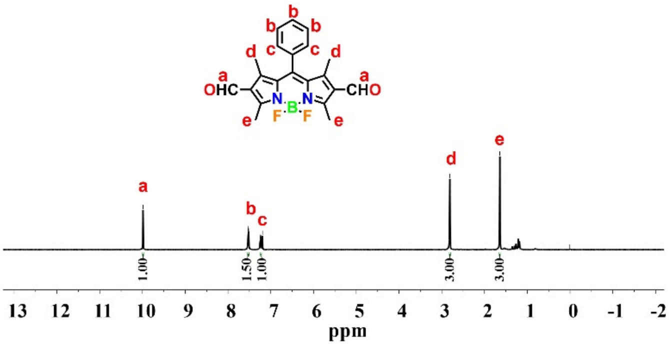


Fig. S10 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **BDP**, δ (ppm): 9.99 (s, 2H), 7.53-7.52 (t, 3H), 7.25~7.22 (d, 2H), 2.81 (s, 6H), 1.64 (s, 6H).

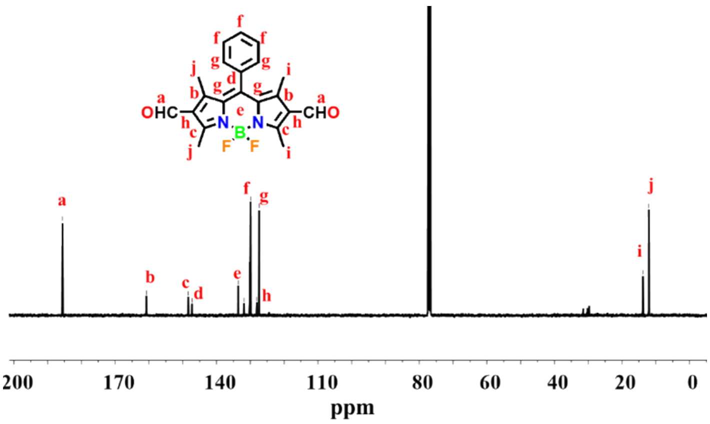


Fig. S11 ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **BDP,** δ (ppm): 185.63, 160.76, 148.39, 147.28, 133.57, 131.88, 130.18, 129.91, 128.08, 127.38, 13.78, 12.05.

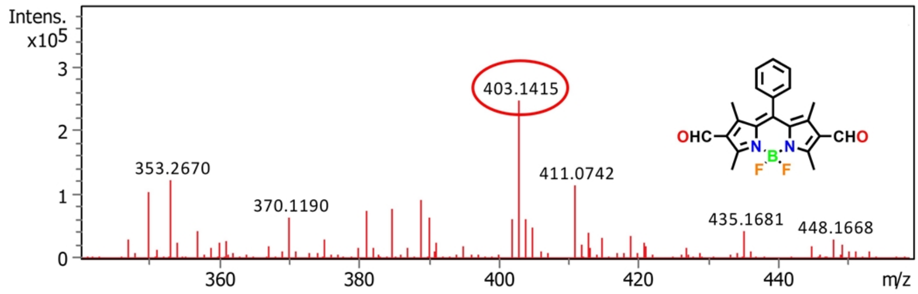


Fig. S12 Mass spectrum (ESI) of **BDP**. *m*/*z* calcd for $[C_{20}H_{19}BF_2N_2O+Na]^+$ 403.1400, found, 403.1415.

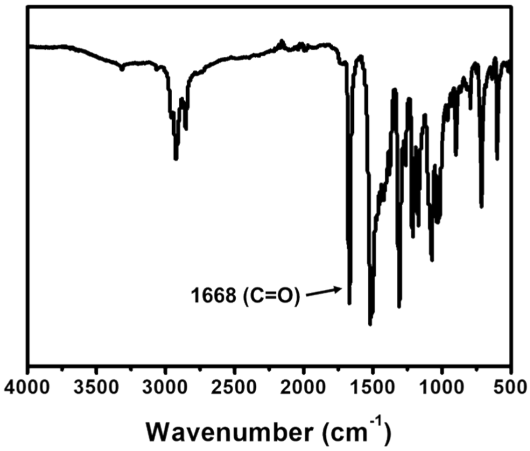


Fig. S13 FTIR spectrum of **BDP** (KBr, cm^{-1}): 2923 (w), 2852 (w), 1668 (s), 1520 (s), 1423 (m), 1307 (s), 1213 (m), 1172 (m), 1072 (s), 1033 (m), 899 (w), 794 (w), 713 (m), 600 (w).

2. Characterization of BCOF and BCOF-Cl

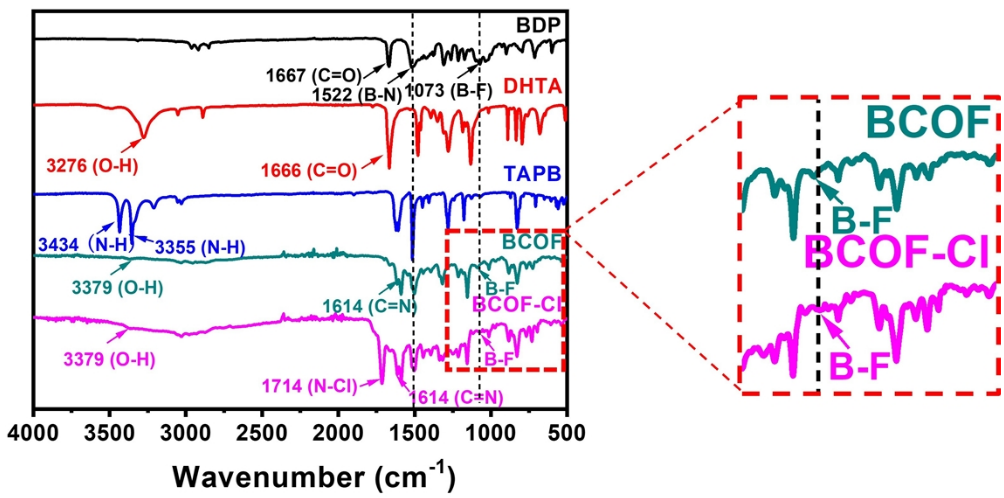


Fig. S14 FTIR spectra (KBr, cm^{-1}) of **BCOF-Cl, BCOF,** and its starting materials.

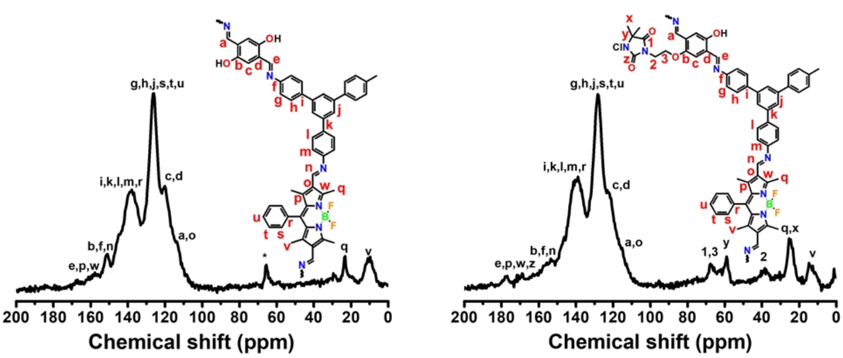


Fig. S15 ^{13}C CP-MAS NMR spectra (100 MHz, ppm): **BCOF** (left): δ 157.7, 150.9, 137.7, 126.5, 120.1, 113.3, 22.9, 10.4. **BCOF-Cl** (right): δ 163.7, 153.9, 139.4, 127.6, 122.5, 115.7, 68.0, 59.2, 38.5, 24.7, 14.5.

Table S1. Fractional atomic coordinates for the unit cell of **BCOF.**
AA stacking mode, space group: $P1$
a=37.6111 Å, b=37.0927 Å, c=4.3181 Å
α=90.0°, β=90.0°,γ=120.0°, R_{wp}=7.84% and R_p=6.13%

Atom	x	y	z	Atom	x	y	z
C1	3.24471	0.82755	0.15851	F51	3.34442	0.57480	-0.77532
C2	3.20292	0.79992	0.21179	N52	3.47091	0.52822	-0.46942
C3	3.18358	0.75918	0.09558	C53	3.49198	0.51103	-0.30451
C4	3.20673	0.74632	-0.07917	C54	3.46965	0.47029	-0.19218
C5	3.24859	0.77345	-0.13675	C55	3.48927	0.45312	-0.02324
C6	3.26720	0.81391	-0.01560	C56	3.53155	0.47656	0.03771
C7	3.26458	0.87070	0.27793	C57	3.55381	0.51747	-0.07534
C8	3.27305	0.75965	-0.31856	C58	3.53426	0.53460	-0.24459
C9	3.13939	0.73042	0.15586	C59	3.55256	0.45834	0.21329
C10	3.30732	0.89668	0.25875	C60	3.53131	0.41648	0.30542
C11	3.32590	0.93793	0.35945	C61	3.55142	0.39851	0.46021
C12	3.30198	0.95394	0.48109	C62	3.59357	0.42310	0.52039
C13	3.25945	0.92808	0.50308	C63	3.61536	0.46510	0.43328
C14	3.24089	0.88674	0.40371	C64	3.59456	0.48233	0.27976
C15	3.11629	0.74389	0.32516	C65	3.66009	0.49032	0.48514
C16	3.07451	0.71710	0.37909	C66	3.52907	0.35376	0.54290
C17	3.05505	0.67620	0.26486	C67	3.68384	0.47103	0.51806
C18	3.07795	0.66256	0.09748	C68	3.72649	0.49494	0.54572
C19	3.11979	0.68942	0.04336	C69	3.74601	0.53859	0.54360
C20	3.25455	0.71975	-0.45102	C70	3.72234	0.55786	0.51776
C21	3.27812	0.70649	-0.61367	C71	3.67973	0.53395	0.48709
C22	3.32063	0.73310	-0.64658	C72	3.48680	0.32920	0.48607
C23	3.33905	0.77289	-0.51711	C73	3.46624	0.28648	0.54618
C24	3.31549	0.78614	-0.35564	C74	3.48767	0.26756	0.66464
N25	3.34631	0.71956	-0.78855	C75	3.52964	0.29198	0.72552
C26	3.33268	0.68433	-0.93049	C76	3.55017	0.33474	0.66621
C27	3.52702	0.77990	-1.27669	N77	3.78978	0.56399	0.55319
C28	3.49370	0.73935	-1.25959	N78	3.46832	0.22335	0.70098
C29	3.49426	0.70977	-1.05956	C79	3.81421	0.54943	0.50218
C30	3.52899	0.72225	-0.87396	C80	3.85903	0.57664	0.50512
C31	3.56277	0.76251	-0.89415	C81	3.42915	0.19863	0.66861
C32	3.56173	0.79141	-1.09517	C82	3.41086	0.15316	0.68074
C33	3.45698	0.66762	-1.03380	C83	3.88439	0.56252	0.38060
C34	3.41596	0.66282	-1.09347	C84	3.92677	0.58944	0.36265
N35	3.38245	0.62512	-1.21224	C85	3.94446	0.63031	0.47421
B36	3.37593	0.58560	-1.02570	C86	3.91923	0.64399	0.60791
N37	3.41650	0.59178	-0.89794	C87	3.87675	0.61736	0.61965
C38	3.45589	0.63071	-0.93762	C88	3.36817	0.12727	0.65506
C39	3.40240	0.68914	-0.98631	C89	3.35126	0.08419	0.63070
C40	3.36105	0.67087	-1.04713	C90	3.37648	0.06637	0.63602
C41	3.34907	0.63348	-1.19387	C91	3.41904	0.09216	0.67212
C42	3.42413	0.56321	-0.77556	C92	3.43601	0.13527	0.69203
C43	3.46855	0.58218	-0.73654	C93	3.98875	0.65923	0.44052
C44	3.48685	0.62232	-0.85146	C94	3.35908	0.02163	0.57824
C45	3.48970	0.56517	-0.58968	N95	3.31978	-0.00339	0.56070
C46	3.42664	0.72718	-0.79321	N96	4.01238	0.64858	0.29673
C47	3.30586	0.60406	-1.29029	O97	3.93566	0.68362	0.72076
C48	3.53207	0.64850	-0.89906	O98	3.86793	0.52298	0.26586
C49	3.39378	0.51799	-0.73390	O99	3.44444	0.07566	0.67784
F50	3.35754	0.54714	-1.22555	O100	3.34286	0.14383	0.64265

H101	3.18400	0.81041	0.35188	H132	3.40967	0.50180	-0.62465
H102	3.19156	0.71337	-0.17679	H133	3.38071	0.50336	-0.96883
H103	3.30123	0.83640	-0.05813	H134	3.36781	0.51430	-0.57644
H104	3.32716	0.88414	0.16035	H135	3.43526	0.45090	-0.23818
H105	3.36065	0.95877	0.34309	H136	3.47093	0.41980	0.06640
H106	3.23971	0.94068	0.60247	H137	3.58818	0.53702	-0.02914
H107	3.20621	0.86570	0.42441	H138	3.55264	0.56788	-0.33489
H108	3.13164	0.77699	0.42003	H139	3.49710	0.39643	0.25482
H109	3.05604	0.72840	0.51639	H140	3.61062	0.40896	0.64197
H110	3.06252	0.62938	0.00431	H141	3.61180	0.51643	0.20656
H111	3.13829	0.67810	-0.09315	H142	3.66834	0.43562	0.52237
H112	3.22005	0.69788	-0.42634	H143	3.74557	0.47901	0.57013
H113	3.26284	0.67402	-0.71991	H144	3.73780	0.59327	0.52164
H114	3.37353	0.79477	-0.54303	H145	3.66063	0.54986	0.46339
H115	3.33069	0.81877	-0.25224	H146	3.46896	0.34411	0.39007
H116	3.29827	0.66320	-0.96682	H147	3.43190	0.26681	0.49908
H117	3.52583	0.80352	-1.43883	H148	3.54731	0.27703	0.82410
H118	3.46543	0.72981	-1.40947	H149	3.58437	0.35454	0.71794
H119	3.53005	0.69942	-0.70270	H150	3.80103	0.51484	0.45371
H120	3.59114	0.77172	-0.74641	H151	3.40807	0.21205	0.62973
H121	3.58919	0.82432	-1.11069	H152	3.94730	0.57823	0.25652
H122	3.52461	0.58387	-0.57256	H153	3.85618	0.62871	0.72306
H123	3.44595	0.75495	-0.95032	H154	3.31663	0.06318	0.60622
H124	3.44766	0.72210	-0.63136	H155	3.47062	0.15627	0.71772
H125	3.40481	0.73350	-0.65058	H156	4.00311	0.69192	0.54206
H126	3.29854	0.57068	-1.24921	H157	3.38028	0.00818	0.54768
H127	3.30212	0.60868	-1.54669	H158	3.91090	0.68785	0.82312
H128	3.28397	0.61039	-1.14854	H159	3.83427	0.50578	0.30659
H129	3.53855	0.66002	-1.14874	H160	3.47292	0.09692	0.80596
H130	3.54731	0.62918	-0.84951	H161	3.35735	0.17405	0.76719
H131	3.54490	0.67631	-0.73531				

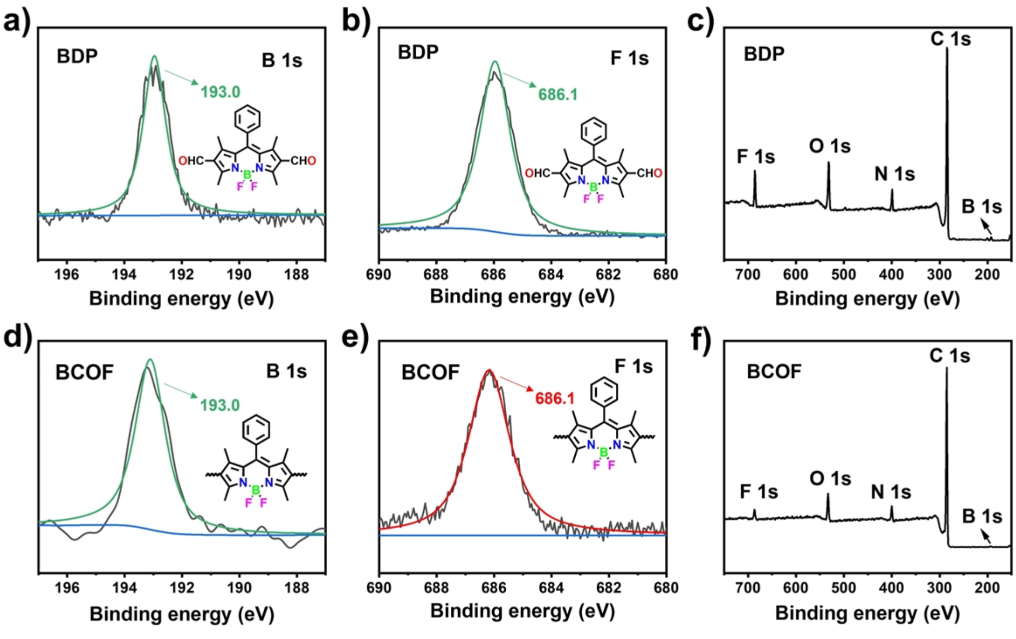


Fig. S16 XPS spectra of BDP and **BCOF**.

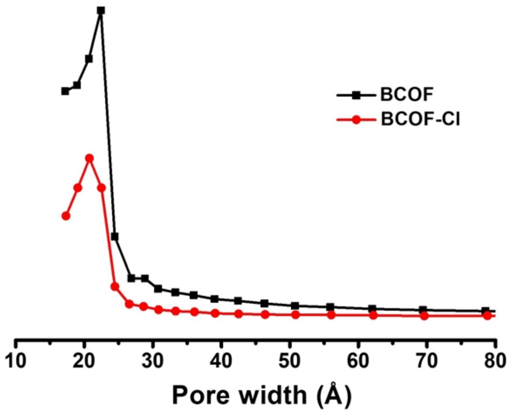


Fig. S17 Pore size distribution of **BCOF** (23.5 Å) and **BCOF-Cl** (21 Å), respectively.

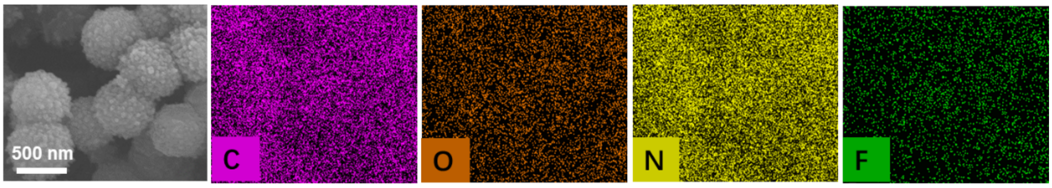


Fig. S18 SEM-EDX elemental mapping images of **BCOF**.

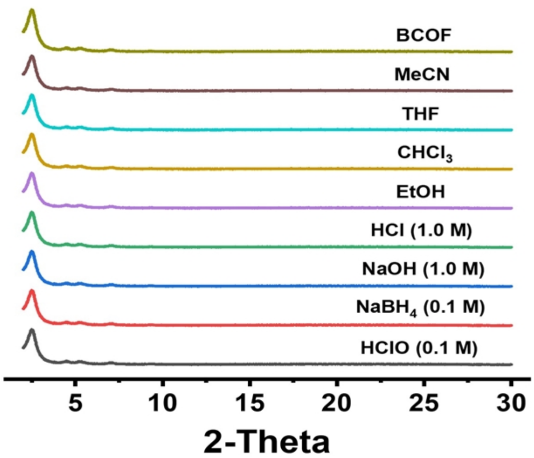


Fig. S19 PXRD patterns of **BCOF** before and after soaking in different media for 24 h.

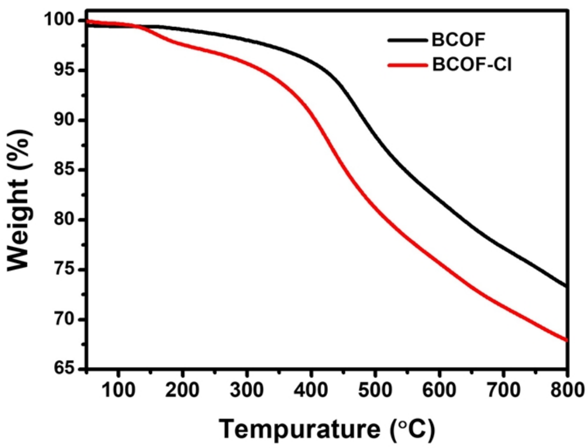


Fig. S20 TGA traces of **BCOF** and **BCOF-Cl**.

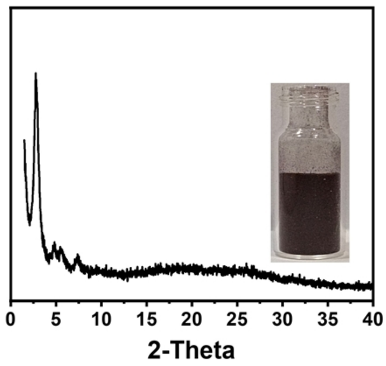


Fig. S21 PXRD patterns of **BCOF** obtained from gram-scale synthesis, with sample photograph in the inset.

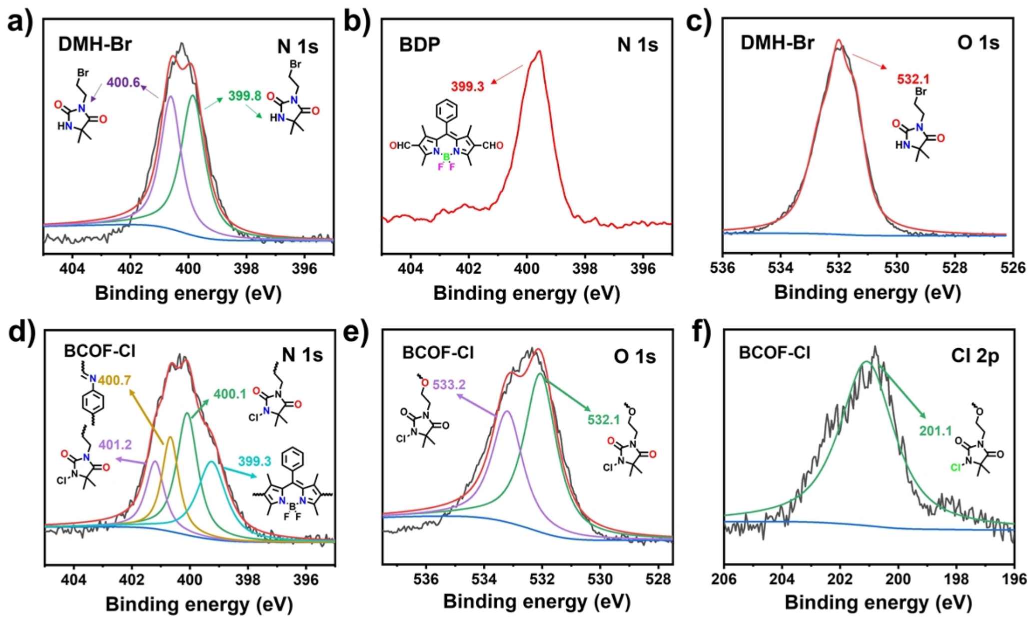


Fig. S22 XPS spectra of BDP, DMH-Br and **BCOF-Cl**.

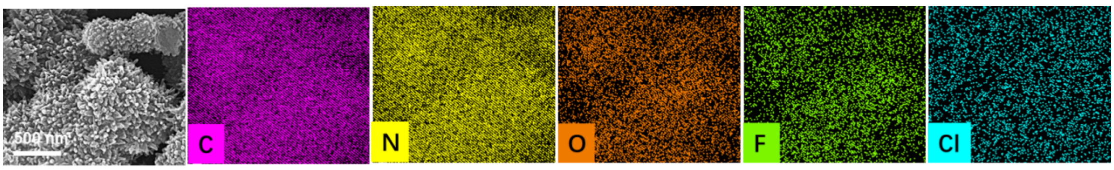


Fig. S23 SEM-EDX elemental mapping images of **BCOF-Cl**.

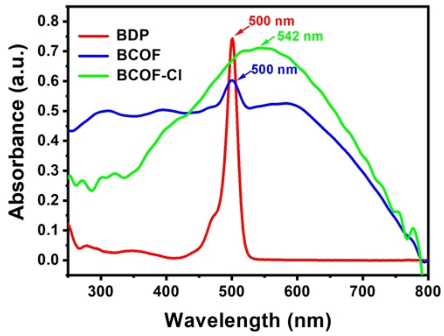


Fig. S24 UV-Vis spectra of **BCOF**, **BCOF-Cl**, and BDP.

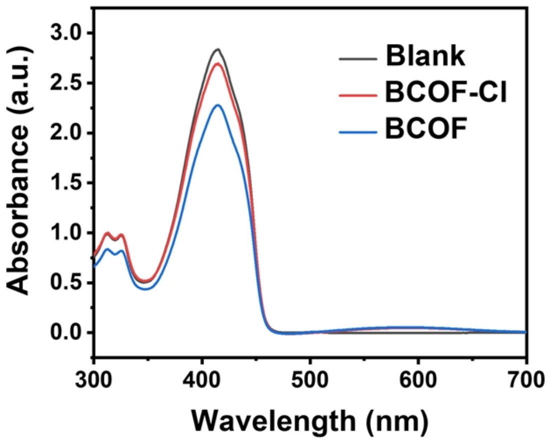


Fig. S25 UV-Vis spectra of the DPBF solution treated with **BCOF**, **BCOF-Cl**, and the blank group without COFs. Under dark conditions, 5 mL of **BCOF-Cl** (10.0 mg) or **BCOF** (9 mg) dispersion in DMF was mixed with 5 mL of 1,3-diphenylisobenzofuran (DPBF) (5.0 mM) in DMF, after adsorption experiments for the same time intervals (1 min), the samples were centrifuged and 1.0 mL of the mother liquor was diluted in a quartz dish to 2.5 mL. The absorbance of the sample was measured at 414 nm. The same concentration of DPBF solution without COF was used as a control.

3. Antibacterial performance

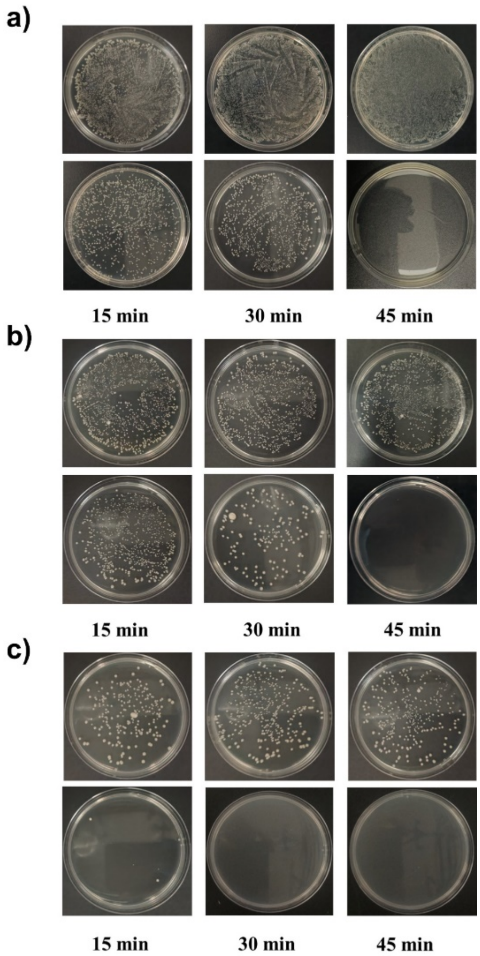


Fig. S26 Photographs of bacterial culture plates of *E. coli* with different initial doses (5.0, 50 and 500 μL, fixed concentration of 10^8 CFU mL^{-1}) treated with **BCOF-Cl** under different exposure times to visible light (52 mW cm^{-2}).

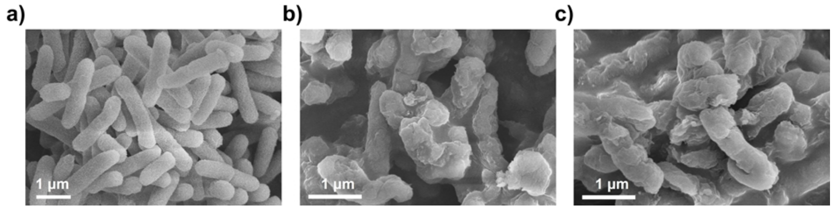


Fig. S27 SEM images of *E. coli* after different treatment: a) the control group, b) treated with **BCOF-Cl** under visible light irradiation (52 mW cm^{-2}), and c) treated with **BCOF-Cl** under sunlight irradiation (50-56 mW cm^{-2}).

Table S2. Ion chromatographic measurement of elemental chlorine in **BCOF-Cl** before and after each antimicrobial cycle.

Antimicrobial cycle		1_{st}	2_{st}	3_{st}	4_{st}	5_{st}
Chlorine, wt%	before	1.69	1.63	1.57	1.61	1.59
	after	0.17	0.13	0.09	0.11	0.12

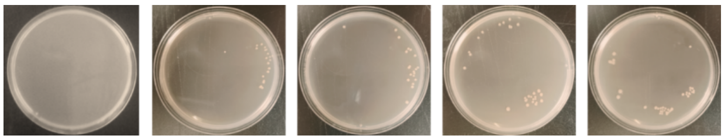


Fig. S28 The photographs of *E. coli* after each antimicrobial cycle (500 uL×10^8 CFU mL^{-1}, 1.0 mg of **BCOF-Cl**, visible light irradiation, λ >400 nm, 52 mW cm^{-2}, 45 min).

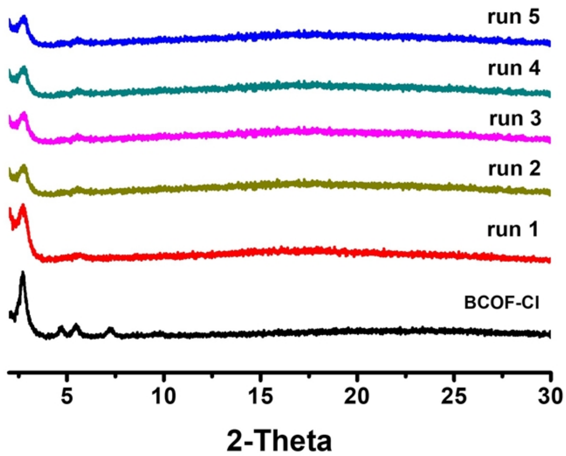


Fig. S29 PXRD patterns of **BCOF-Cl** after each antimicrobial cycle.

4. Characterization of BCOF-Cl@chitosan aerogel

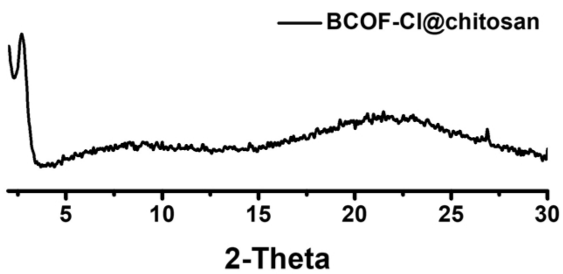


Fig. S30 PXRD pattern of the **BCOF-Cl@chitosan** aerogel.

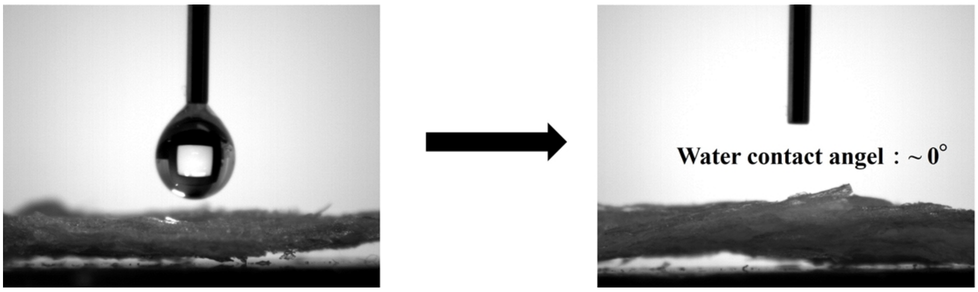


Fig. S31 WCA images of **BCOF-Cl@chitosan** aerogel. The superhydrophilic nature of the samples was demonstrated by the rapid penetration of water droplets within 1 second.

5. Continuous flow-through water disinfection over BCOF-Cl@chitosan

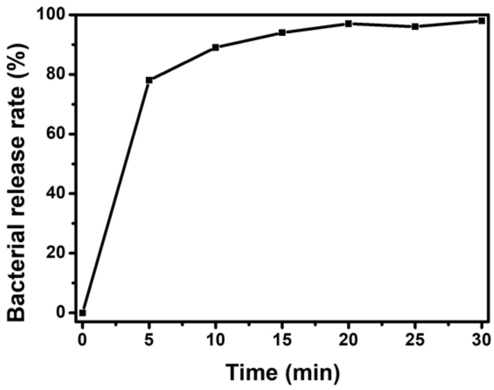


Fig. S32 Bacterial release behavior of **BCOF-Cl@chitosan** aerogel against *E. coli* via anti-fouling experiment. General procedure: 10 μL of the diluted *E. coli* solution (10^8 CFU mL^{-1}) was dripped on the **BCOF-Cl@chitosan** aerogel (5.0 mg), and then it was incubated at 37 °C for 5 h to fix the bacteria. The sample was then immersed in PBS buffer to access the released bacteria from the samples at each time point by the plate count method.[2]

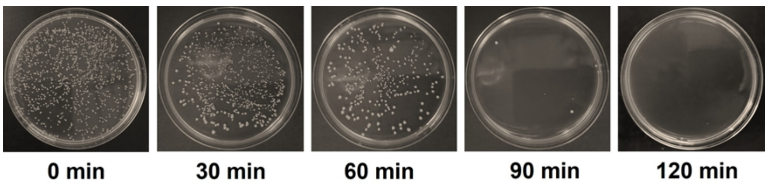


Fig. S33 Photographs of bacterial culture plates of *E. coli* treated with **BCOF-Cl@chitosan** aerogel upon sunlight irradiation (50-56 mW cm^{-2}) within 2 h.

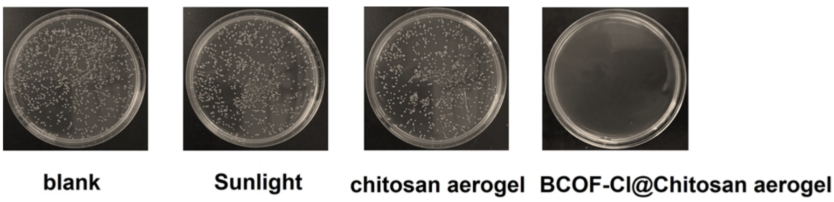


Fig. S34 Comparison of photographs of bacterial culture plates of *E. coli* treated with different materials after exposure to sunlight irradiation (50-56 mW cm^{-2}) for 2 h.

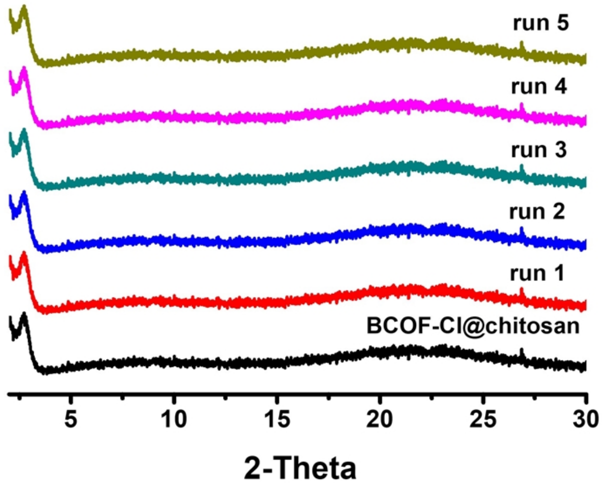


Fig. S35 PXRD pattern of the **BCOF-Cl@chitosan** aerogel each antimicrobial cycle in the continuous operation of sunlight-powered water sterilization.

6. References

[1] J. Kang, F. Huo, Y. Yue, Y. Wen, J. Chao, Y. Zhang and C. Yin, , *Dyes and Pigments*, 2017, **136,** 852.

[2] W.-X. Wu, F. Li , B.-J. Yao, L.-G. Ding , J.-L. Kan, F. Liu, G.-Y. Zhao, S. Wang, Y.-B. Dong, *J Hazard. Mater.,* 2022, **433,** 128831.