

# Two-Dimensional Salen-Based Covalent Organic Frameworks with High Electronegative Groups as Separators for High Stability Lithium-Sulfur Battery

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## Section A. Material and methods

All commercially available reagents and solvents were used as received without further purification, unless otherwise noted. 2, 4, 6-tris(4-aminophenyl)-1, 3, 5-triazine (TAPT) was purchased from Alfa, Salen was purchased from Kayulin Shanghai. All solvents used, pure sulfur, conductive carbon black, and polyvinylidene fluoride (PVDF) were purchased from Aladdin.

Fourier transforms Infrared (FT-IR) spectra were recorded on a Perkin-Elmer model FT-IR-frontier infrared spectrometer. For all FT-IR tests, a small amount of sample can be directly mixed with potassium bromide and ground into a powder, compressed, and the pressed product can be directly tested. The solid-state UV-visible analyzer was used for Jasco V-770 spectrometer Solid-state.  $^{13}\text{C}$  cross-polarization/magic angle spinning nuclear magnetic resonance (CP/MAS NMR) analysis was conducted using AVANCEIII/WB-400. Field-emission scanning electron microscopy (FE-SEM) images were performed on a JEOL model JSM-6700 operating at an accelerating voltage of 5.0 kV. Powder X-ray diffraction (PXRD) data were recorded on a Rigaku model RINT Ultima III diffractometer by depositing powder on glass substrate, from  $2\theta = 2^\circ$  up to  $30^\circ$  with  $0.02^\circ$  increment. TGA analysis was carried out by using a Q5000IR analyzer (TA Instruments) with an automated vertical overhead thermobalance. Before measurement, the samples were heated at a rate of  $10 \text{ }^\circ\text{C min}^{-1}$  under a nitrogen atmosphere. X-ray photoelectron spectra (XPS) were recorded on an ESCALAB250Xielectron spectrometer (Thermo Fisher Scientific Inc., Waltham, MA, USA). Nitrogen sorption isotherms were measured at 77 K with Bel Japan Inc. Model BELSORP-max analyzer. Before measurement, the samples were degassed in vacuum at  $100 \text{ }^\circ\text{C}$  for more than 10 h. The Brunauer-Emmett-Teller (BET) method was utilized to calculate the specific surface areas and pore volume. The nonlocal density functional theory (NLDFT) method was applied for the estimation of pore size and pore size distribution.

All processes were carried out in an Ar-filled glovebox ( $\text{H}_2\text{O} < 0.1 \text{ ppm}$ ,  $\text{O}_2 < 0.1 \text{ ppm}$ ). The battery test system (LANHE CT2001A, Wuhan LAND Electronics Co.) was employed to evaluate the cycling performance with a voltage range from 1.8

to 2.8 V. CV (1.7-2.8V, 0.1 mV s<sup>-1</sup>), electrochemical impedance spectra (EIS) (10<sup>-1</sup>-10<sup>5</sup> Hz) and I-t curves were measured on CHI 660E, Chenhua.

The conductivity of Li<sup>+</sup> in the separator can be calculated using the EIS of a stainless steel symmetrical battery and formula (1-1):

$$\sigma = \frac{L}{RA} \#( -1 )$$

In equation (1-1), L and A represent the thickness and area of the separator, respectively, and R is the bulk ohmic resistance of the electrolyte.

Using the constant potential polarization method, the I-t curve of Li/separator/Li battery structure was tested, with a polarization voltage of 0.02 V and a polarization time of 1000 s. The Li<sup>+</sup> migration number was calculated using formula (1-2):

$$t_{Li^+} = \frac{I_S(\Delta V - I_0 R_0)}{I_0(\Delta V - I_S R_S)} \#(1 - 2)$$

In equation (1-2), Δ V represents the constant voltage applied, R<sub>0</sub> and R<sub>S</sub> represent the initial resistance and polarization resistance, respectively, and I<sub>0</sub> and I<sub>S</sub> represent the initial and steady-state current, respectively.

## Section B. Synthetic procedures

Synthesis of Salen-TAPT-COF:

Salen (21.8 mg), 1,3,5-tris(4-aminophenyl)-1,3,5-triazine (TAPT, 7.1 mg) were added to a 5 mL Pyrex tube, 1,2-dichlorobenzene (0.5 mL), 1,3,5-triethylbenzene (0.5 mL) were added to the Pyrex tube. The above mixture was treated in an ultrasonic instrument for 5 min to evenly disperse, and then an aqueous acetic acid solution (6 M, 0.2 mL) was added. Then the tube was degassed by freezing pump thawing technology for three cycles in a liquid nitrogen bath, sealed under vacuum, and reacted in a oven at 120 °C for 5 days. After the reaction was completed and cooled to room temperature, and the red solid product was separated by centrifugation, washed with THF until the color of the washing solution becomes colorless. Finally, a red solid powder Salen-TAPT-COF was obtained by drying under dynamic vacuum for

12 h at 100 °C, with a yield of 72.3%.

### **Section C. Preparation of separator and its assembly for Li-S batteries**

Preparation of Salen-TAPT-COF/PP separator:

Firstly, the Salen-TAPT -COF composite is mixed with polyvinylidene fluoride (PVDF) and Super-P in a weight ratio of 7:1:2, and the mixture is ground in a mortar for 30 minutes. Then an appropriate amount of N-methylpyrrolidone (NMP) was added to grind into a slurry, the ground slurry was scraped onto the PP membrane using a four-sided sample preparatory, and dry in a vacuum oven at 60 °C for 12 h to obtain a modified Salen-TAPT -COF composite separator.

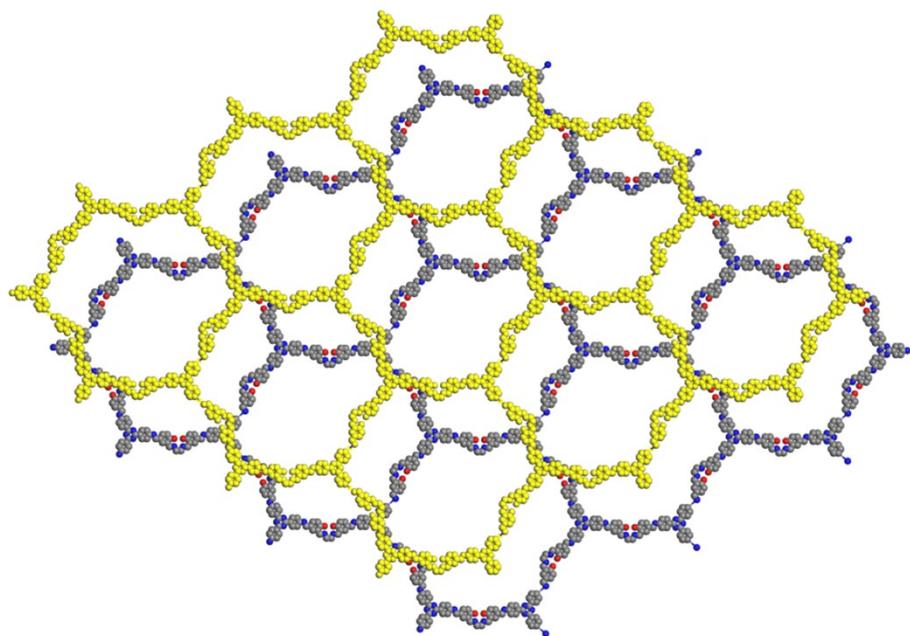
Li-S batteries assembly:

In a glove box filled with argon gas ( $O_2 < 0.01$  ppm,  $H_2O < 0.01$  ppm), assemble in the following order: a. Put in the cathode shell; b. Put in the cathode pole piece; c. Drop in 40  $\mu$ l of electrolyte, which is a conventional electrolyte containing 1 M LiTFSI and 1 wt% LiNO<sub>3</sub> as the solute, and v(DOL): v(DME) = 1:1 as the solvent; d. put in the diaphragm; e. put in the lithium wafers; f. put in the spacer; g. put in the shrapnel; h. put in the negative shell. The battery was encapsulated using a battery sealer, applying a pressure of about 5 MPa. The electrochemical characteristics of the battery were determined after the battery was left for 10 h.

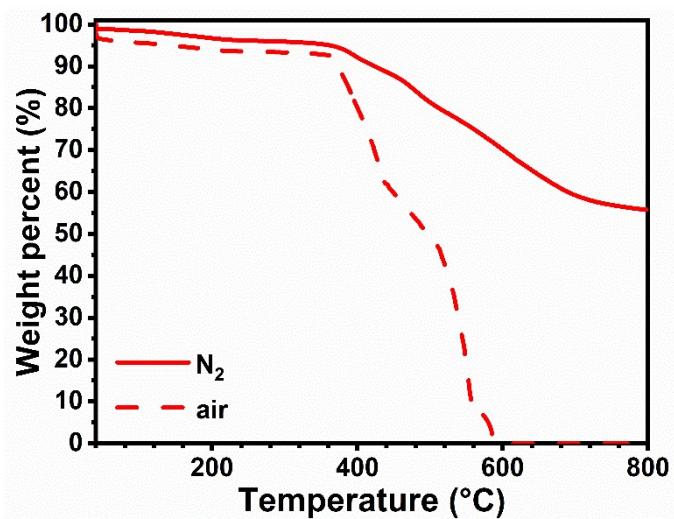
Electrochemical Evaluation

The cells were galvanostatically cycled in the cut-off potential of 1.8 – 2.7 V on a Land battery tester under different C-rates. The cyclic voltammetry (CV) curves were recorded on a CHENHUA electrochemical workstation at a scanning rate of 0.1 mV s<sup>-1</sup>. Electrochemical impedance spectroscopy (EIS) was also performed on a CHENHUA electrochemical workstation with a frequency range of 0.01 to 10<sup>6</sup> Hz.

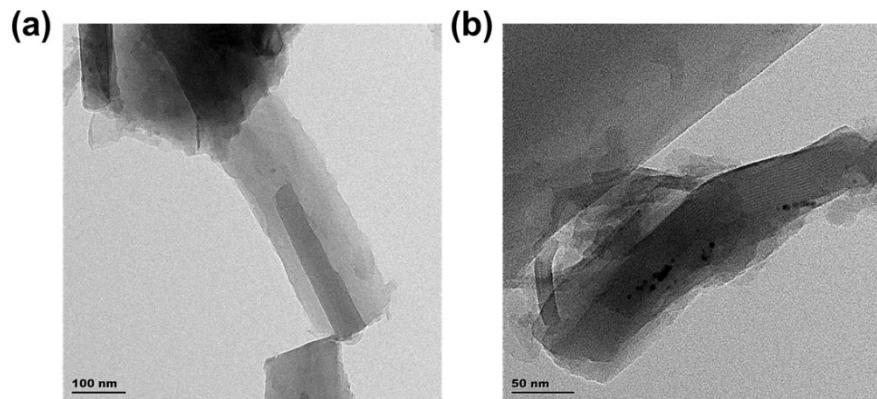
## Section D. Supplementary Figures



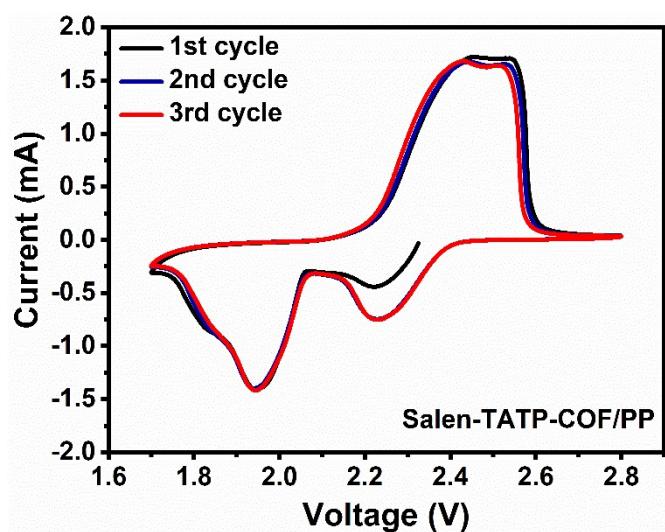
**Fig. S1.** The Top views of the AB stacking structure of Salen-TAPT-COF -COF.



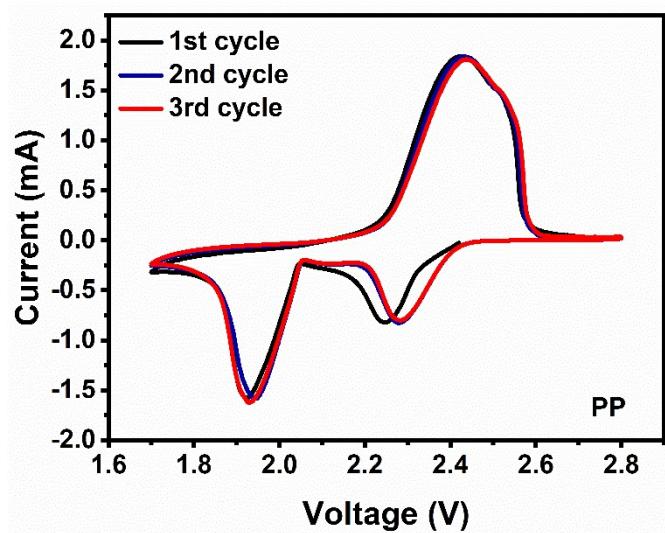
**Fig. S2.** TGA curves of Salen-TAPT-COF under  $N_2$  and air atmosphere.



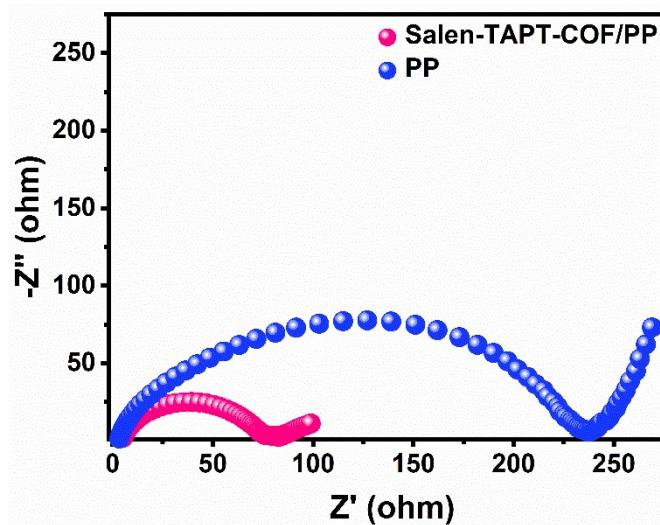
**Fig. S3.** TEM images of Salen-TAPT-COF.



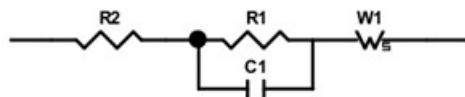
**Fig. S4.** CV curves of Salen-TAPT-COF/PP.



**Fig. S5.** CV curves of PP.



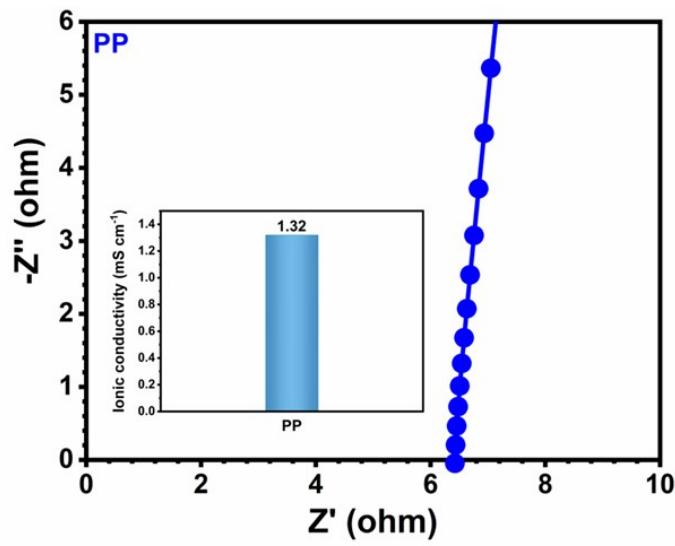
**Fig. S6.** EIS spectra of PP separators and Salen-TAPT-COF modified separators Li-S batteries.



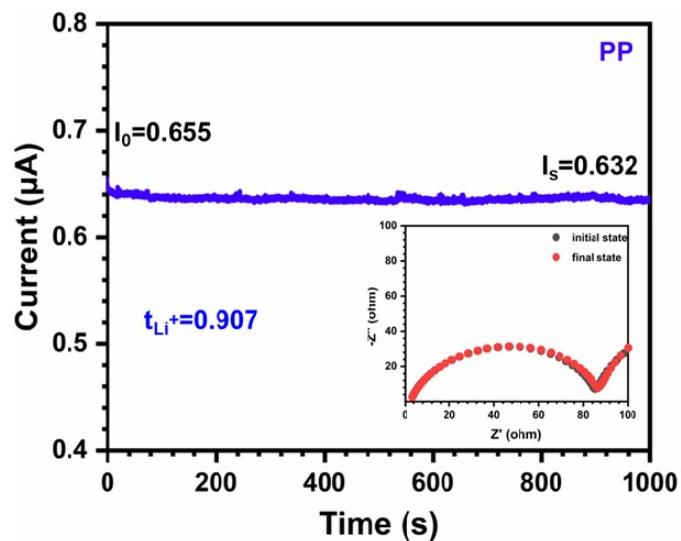
**Fig. S7.** The equivalent circuit spectras of PP separators and Salen-TAPT-COF modified separators Li-S batteries.



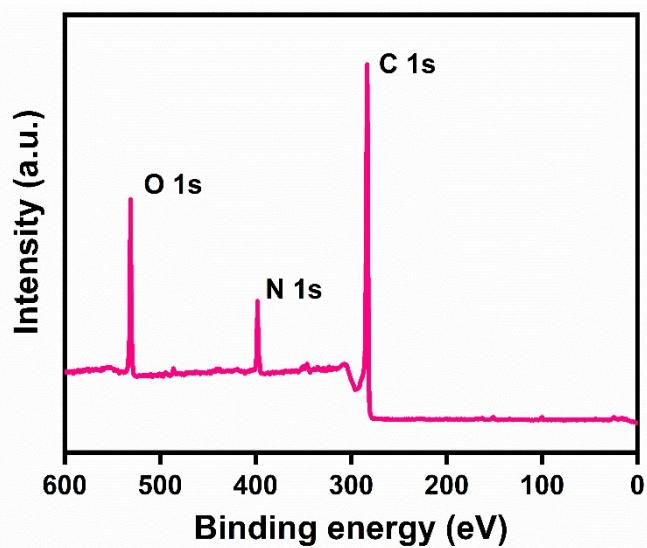
**Fig. S8.** The water contact angle of Salen-TAPT-COF/PP.



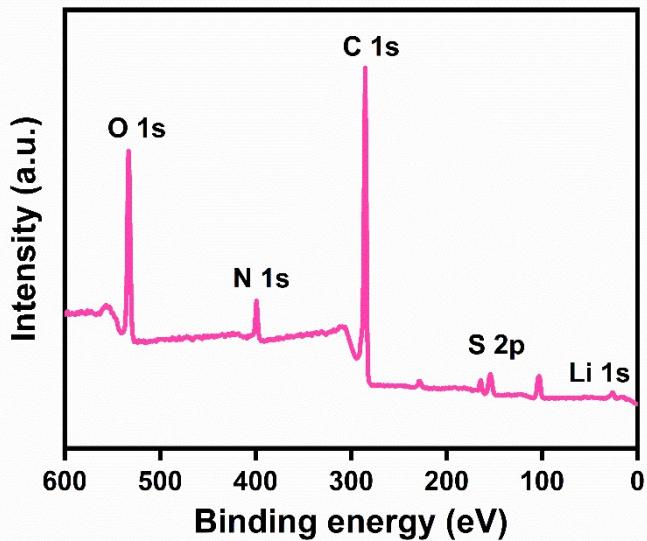
**Fig. S9.** EIS plots of PP separators at 25 °C (inset: ionic conductivities).



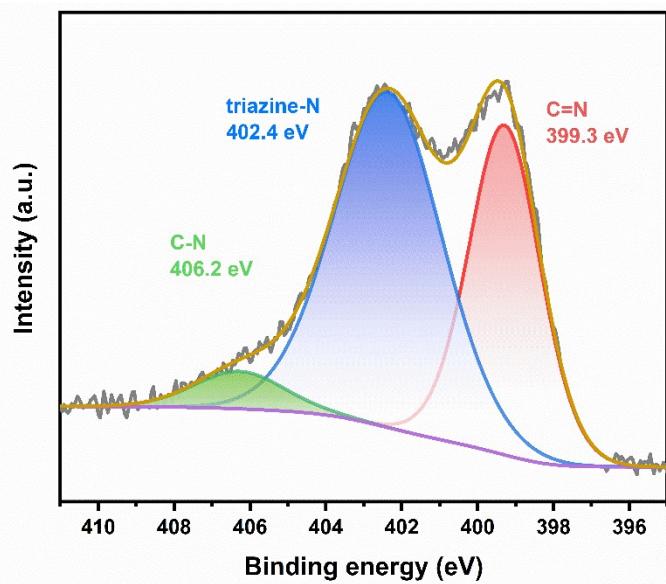
**Fig. S10.** I-t curves of Li/Li symmetric cells with PP separators (insets: EIS plots of the symmetric cells).



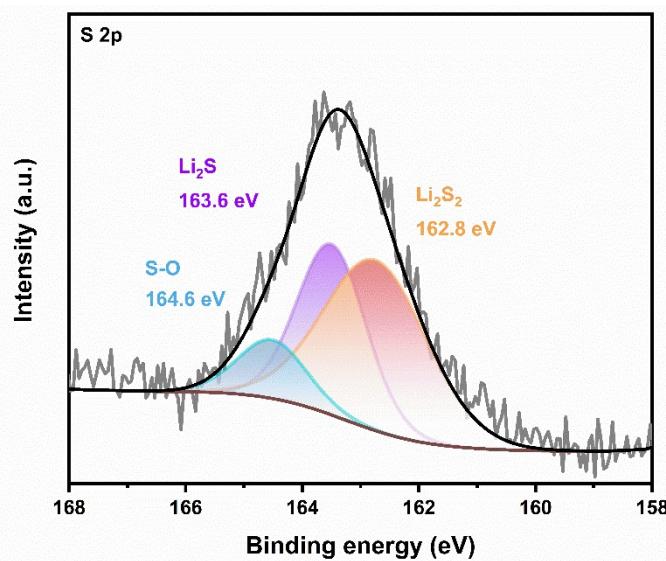
**Fig. S11.** XPS survey spectra of Salen-TAPT-COF before adsorption experiment.



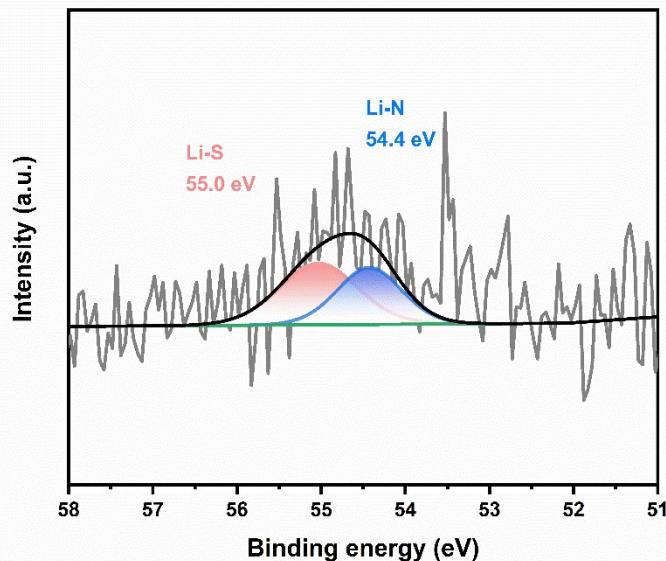
**Fig. S12.** XPS survey spectra of Salen-TAPT-COF after adsorption experiment.



**Fig. S13.** The N 1s XPS spectra of Salen-TAPT-COF.



**Fig. S14.** The S 2P XPS spectra of Salen-TAPT-COF after adsorption experiment.



**Fig. S15.** The Li 1s XPS spectra of Salen-TAPT-COF after adsorption experiment.

### Section E. Supplementary Tables

**Table S1.** Atomistic coordinates of AA stacking for Salen-TAPT-COF optimized by using Materials Studio method.  $a = 55.000 \text{ \AA}$ ,  $b = 55.00 \text{ \AA}$ ,  $c = 5.000 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 120^\circ$ .

N1	N	0.8402	-0.81626	0
C2	C	0.80997	-0.83138	0
N3	N	0.79485	-0.86166	0
C4	C	0.80997	-0.87683	0
N5	N	0.8402	-0.86172	0
C6	C	0.85532	-0.83143	0
C7	C	0.88555	-0.81632	0
C8	C	0.79485	-0.90694	0
C9	C	0.79485	-0.81639	0
C10	C	0.76462	-0.92205	0
C11	C	0.74951	-0.95234	0
C12	C	0.76462	-0.96751	0
C13	C	0.79485	-0.95239	0
C14	C	0.80997	-0.92211	0
C15	C	0.80997	-0.78611	0
C16	C	0.79485	-0.77094	0
C17	C	0.76462	-0.78605	0
C18	C	0.74951	-0.81634	0
C19	C	0.76462	-0.83151	0

C20	C	0.90067	-0.83148	0
C21	C	0.9309	-0.81637	0
C22	C	0.94601	-0.78608	0
C23	C	0.9309	-0.77091	0
C24	C	0.90067	-0.78603	0
N25	N	0.58344	-0.3781	0
C26	C	0.56832	-0.45366	0
C27	C	0.58344	-0.42337	0
C28	C	0.56832	-0.4082	0
C29	C	0.53809	-0.42332	0
C30	C	0.52297	-0.4536	0
C31	C	0.52297	-0.5896	0
C32	C	0.53809	-0.60477	0
C33	C	0.56832	-0.58966	0
C34	C	0.58344	-0.55937	0
C35	C	0.56832	-0.54438	0
C36	C	0.43228	-0.54441	0
C37	C	0.40205	-0.55952	0
C38	C	0.38693	-0.58963	0
C39	C	0.40205	-0.6048	0
C40	C	0.43228	-0.58968	0
C41	C	0.53809	-0.5595	0
C42	C	0.44739	-0.55939	0
C43	C	0.53809	-0.46877	0
C44	C	0.52297	-0.49906	0
N45	N	0.49274	-0.51417	0
C46	C	0.47763	-0.54428	0
N47	N	0.49274	-0.55945	0
C48	C	0.52297	-0.54433	0
N49	N	0.53809	-0.51405	0
C50	C	0.58323	-0.28748	0
C51	C	0.56811	-0.31776	0
C52	C	0.58323	-0.33275	0
C53	C	0.61346	-0.31763	0
C54	C	0.62858	-0.28735	0
C55	C	0.61346	-0.27218	0
C56	C	0.5679	-0.27241	0
N57	N	0.58302	-0.24231	0
C58	C	0.5679	-0.22714	0
O59	O	0.62837	-0.24218	0
C60	C	0.56832	-0.36293	0
C61	C	0.71927	-0.06091	0
O62	O	0.6586	-0.18179	0

C63	C	0.58302	-0.19685	0
N64	N	0.61325	-0.18174	0
C65	C	0.62837	-0.15145	0
C66	C	0.67372	-0.15169	0
C67	C	0.70395	-0.13657	0
C68	C	0.71906	-0.10647	0
C69	C	0.70416	-0.09119	0
C70	C	0.67393	-0.10613	0
C71	C	0.6586	-0.13652	0
C72	C	0.67414	-0.60475	0
C73	C	0.65902	-0.58958	0
C74	C	0.62879	-0.6047	0
C75	C	0.61367	-0.63498	0
C76	C	0.629	-0.65005	0
C77	C	0.65923	-0.63475	0
C78	C	0.70437	-0.58945	0
N79	N	0.71948	-0.60462	0
C80	C	0.74972	-0.58951	0
O81	O	0.67435	-0.64992	0
C82	C	0.61367	-0.58971	0
C83	C	0.76462	-0.74078	0
O84	O	0.70437	-0.68	0
C85	C	0.76483	-0.60468	0
N86	N	0.74972	-0.63478	0
C87	C	0.76483	-0.64995	0
C88	C	0.71948	-0.69517	0
C89	C	0.70437	-0.72545	0
C90	C	0.71927	-0.74073	0
C91	C	0.74951	-0.72561	0
C92	C	0.76483	-0.69522	0
C93	C	0.74972	-0.68023	0
N94	N	0.74951	-0.77088	0
N95	N	0.58344	-0.60483	0
C96	C	0.266	-0.69573	0
C97	C	0.29623	-0.68043	0
C98	C	0.31135	-0.65014	0
C99	C	0.29602	-0.63526	0
C100	C	0.26579	-0.65038	0
C101	C	0.25088	-0.68056	0
C102	C	0.25088	-0.72601	0
N103	N	0.22065	-0.74113	0
C104	C	0.20554	-0.77123	0
O105	O	0.22065	-0.69567	0

C106	C	0.34158	-0.63503	0
C107	C	0.03947	-0.78608	0
O108	O	0.1604	-0.7258	0
C109	C	0.1753	-0.78635	0
N110	N	0.16019	-0.77136	0
C111	C	0.12996	-0.78648	0
C112	C	0.13017	-0.74092	0
C113	C	0.11505	-0.72575	0
C114	C	0.08482	-0.74086	0
C115	C	0.0697	-0.77097	0
C116	C	0.08482	-0.78614	0
C117	C	0.11505	-0.7712	0
N118	N	0.3567	-0.60474	0
N119	N	0.02435	-0.77091	0
N120	N	0.74951	-0.04579	0

**Table S2.** Atomistic coordinates of AB stacking for Salen-TAPT-COF optimized by using Materials Studio method.  $a = 55.000 \text{ \AA}$ ,  $b = 55.000 \text{ \AA}$ ,  $c = 10.000 \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 90^\circ$ ,  $\gamma = 120^\circ$ .

N1	N	0.8402	0.18374	0.25
C2	C	0.80997	0.16862	0.25
N3	N	0.79485	0.13834	0.25
C4	C	0.80997	0.12317	0.25
N5	N	0.8402	0.13828	0.25
C6	C	0.85532	0.16857	0.25
C7	C	0.88555	0.18368	0.25
C8	C	0.79485	0.09306	0.25
C9	C	0.79485	0.18361	0.25
C10	C	0.76462	0.07795	0.25
C11	C	0.74951	0.04766	0.25
C12	C	0.76462	0.03249	0.25
C13	C	0.79485	0.04761	0.25
C14	C	0.80997	0.07789	0.25
C15	C	0.80997	0.21389	0.25
C16	C	0.79485	0.22906	0.25
C17	C	0.76462	0.21395	0.25
C18	C	0.74951	0.18366	0.25
C19	C	0.76462	0.16849	0.25
C20	C	0.90067	0.16852	0.25
C21	C	0.9309	0.18363	0.25
C22	C	0.94601	0.21392	0.25

C23	C	0.9309	0.22909	0.25
C24	C	0.90067	0.21397	0.25
N25	N	0.58344	0.6219	0.25
C26	C	0.56832	0.54634	0.25
C27	C	0.58344	0.57663	0.25
C28	C	0.56832	0.5918	0.25
C29	C	0.53809	0.57668	0.25
C30	C	0.52297	0.5464	0.25
C31	C	0.52297	0.4104	0.25
C32	C	0.53809	0.39523	0.25
C33	C	0.56832	0.41034	0.25
C34	C	0.58344	0.44063	0.25
C35	C	0.56832	0.45562	0.25
C36	C	0.43228	0.45559	0.25
C37	C	0.40205	0.44048	0.25
C38	C	0.38693	0.41037	0.25
C39	C	0.40205	0.3952	0.25
C40	C	0.43228	0.41032	0.25
C41	C	0.53809	0.4405	0.25
C42	C	0.44739	0.44061	0.25
C43	C	0.53809	0.53123	0.25
C44	C	0.52297	0.50094	0.25
N45	N	0.49274	0.48583	0.25
C46	C	0.47763	0.45572	0.25
N47	N	0.49274	0.44055	0.25
C48	C	0.52297	0.45567	0.25
N49	N	0.53809	0.48595	0.25
C50	C	0.58323	0.71252	0.25
C51	C	0.56811	0.68224	0.25
C52	C	0.58323	0.66725	0.25
C53	C	0.61346	0.68237	0.25
C54	C	0.62858	0.71265	0.25
C55	C	0.61346	0.72782	0.25
C56	C	0.5679	0.72759	0.25
N57	N	0.58302	0.75769	0.25
C58	C	0.5679	0.77286	0.25
O59	O	0.62837	0.75782	0.25
C60	C	0.56832	0.63707	0.25
C61	C	0.71927	0.93909	0.25
O62	O	0.6586	0.81821	0.25
C63	C	0.58302	0.80315	0.25
N64	N	0.61325	0.81826	0.25
C65	C	0.62837	0.84855	0.25

C66	C	0.67372	0.84831	0.25
C67	C	0.70395	0.86343	0.25
C68	C	0.71906	0.89353	0.25
C69	C	0.70416	0.90881	0.25
C70	C	0.67393	0.89387	0.25
C71	C	0.6586	0.86348	0.25
C72	C	0.67414	0.39525	0.25
C73	C	0.65902	0.41042	0.25
C74	C	0.62879	0.3953	0.25
C75	C	0.61367	0.36502	0.25
C76	C	0.629	0.34995	0.25
C77	C	0.65923	0.36525	0.25
C78	C	0.70437	0.41055	0.25
N79	N	0.71948	0.39538	0.25
C80	C	0.74972	0.41049	0.25
O81	O	0.67435	0.35008	0.25
C82	C	0.61367	0.41029	0.25
C83	C	0.76462	0.25922	0.25
O84	O	0.70437	0.32	0.25
C85	C	0.76483	0.39532	0.25
N86	N	0.74972	0.36522	0.25
C87	C	0.76483	0.35005	0.25
C88	C	0.71948	0.30483	0.25
C89	C	0.70437	0.27455	0.25
C90	C	0.71927	0.25927	0.25
C91	C	0.74951	0.27439	0.25
C92	C	0.76483	0.30478	0.25
C93	C	0.74972	0.31977	0.25
N94	N	0.74951	0.22912	0.25
N95	N	0.58344	0.39517	0.25
C96	C	0.266	0.30427	0.25
C97	C	0.29623	0.31957	0.25
C98	C	0.31135	0.34986	0.25
C99	C	0.29602	0.36474	0.25
C100	C	0.26579	0.34962	0.25
C101	C	0.25088	0.31944	0.25
C102	C	0.25088	0.27399	0.25
N103	N	0.22065	0.25887	0.25
C104	C	0.20554	0.22877	0.25
O105	O	0.22065	0.30433	0.25
C106	C	0.34158	0.36497	0.25
C107	C	0.03947	0.21392	0.25
O108	O	0.1604	0.2742	0.25

C109	C	0.1753	0.21365	0.25
N110	N	0.16019	0.22864	0.25
C111	C	0.12996	0.21352	0.25
C112	C	0.13017	0.25908	0.25
C113	C	0.11505	0.27425	0.25
C114	C	0.08482	0.25914	0.25
C115	C	0.0697	0.22903	0.25
C116	C	0.08482	0.21386	0.25
C117	C	0.11505	0.2288	0.25
N118	N	0.3567	0.39526	0.25
N119	N	0.02435	0.22909	0.25
N120	N	0.74951	0.95421	0.25
N121	N	1.25224	0.34847	0.75
C122	C	1.22201	0.33336	0.75
N123	N	1.2069	0.30307	0.75
C124	C	1.22201	0.2879	0.75
N125	N	1.25224	0.30302	0.75
C126	C	1.26736	0.3333	0.75
C127	C	1.29759	0.34842	0.75
C128	C	1.2069	0.2578	0.75
C129	C	1.2069	0.34834	0.75
C130	C	1.17666	0.24268	0.75
C131	C	1.16155	0.2124	0.75
C132	C	1.17666	0.19723	0.75
C133	C	1.2069	0.21234	0.75
C134	C	1.22201	0.24263	0.75
C135	C	1.22201	0.37863	0.75
C136	C	1.2069	0.3938	0.75
C137	C	1.17666	0.37868	0.75
C138	C	1.16155	0.3484	0.75
C139	C	1.17666	0.33323	0.75
C140	C	1.31271	0.33325	0.75
C141	C	1.34294	0.34836	0.75
C142	C	1.35806	0.37865	0.75
C143	C	1.34294	0.39382	0.75
C144	C	1.31271	0.3787	0.75
N145	N	0.99548	0.78663	0.75
C146	C	0.98036	0.71108	0.75
C147	C	0.99548	0.74136	0.75
C148	C	0.98036	0.75653	0.75
C149	C	0.95013	0.74142	0.75
C150	C	0.93502	0.71113	0.75
C151	C	0.93502	0.57513	0.75

C152	C	0.95013	0.55996	0.75
C153	C	0.98036	0.57508	0.75
C154	C	0.99548	0.60536	0.75
C155	C	0.98036	0.62035	0.75
C156	C	0.84432	0.62033	0.75
C157	C	0.81409	0.60521	0.75
C158	C	0.79897	0.57511	0.75
C159	C	0.81409	0.55994	0.75
C160	C	0.84432	0.57505	0.75
C161	C	0.95013	0.60523	0.75
C162	C	0.85944	0.60534	0.75
C163	C	0.95013	0.69596	0.75
C164	C	0.93502	0.66568	0.75
N165	N	0.90478	0.65056	0.75
C166	C	0.88967	0.62046	0.75
N167	N	0.90478	0.60529	0.75
C168	C	0.93502	0.6204	0.75
N169	N	0.95013	0.65069	0.75
C170	C	0.99527	0.87726	0.75
C171	C	0.98015	0.84697	0.75
C172	C	0.99527	0.83198	0.75
C173	C	1.0255	0.8471	0.75
C174	C	1.04062	0.87739	0.75
C175	C	1.0255	0.89256	0.75
C176	C	0.97994	0.89232	0.75
N177	N	0.99506	0.92243	0.75
C178	C	0.97994	0.93759	0.75
O179	O	1.04041	0.92255	0.75
C180	C	0.98036	0.8018	0.75
C181	C	1.13132	1.10383	0.75
O182	O	1.07064	0.98294	0.75
C183	C	0.99506	0.96788	0.75
N184	N	1.02529	0.983	0.75
C185	C	1.04041	1.01328	0.75
C186	C	1.08576	1.01305	0.75
C187	C	1.11599	1.02816	0.75
C188	C	1.13111	1.05827	0.75
C189	C	1.1162	1.07354	0.75
C190	C	1.08597	1.05861	0.75
C191	C	1.07064	1.02822	0.75
C192	C	1.08618	0.55998	0.75
C193	C	1.07106	0.57515	0.75
C194	C	1.04083	0.56004	0.75

C195	C	1.02571	0.52975	0.75
C196	C	1.04104	0.51469	0.75
C197	C	1.07127	0.52998	0.75
C198	C	1.11641	0.57528	0.75
N199	N	1.13153	0.56011	0.75
C200	C	1.16176	0.57523	0.75
O201	O	1.08639	0.51482	0.75
C202	C	1.02571	0.57502	0.75
C203	C	1.17666	0.42395	0.75
O204	O	1.11641	0.48474	0.75
C205	C	1.17687	0.56006	0.75
N206	N	1.16176	0.52996	0.75
C207	C	1.17687	0.51479	0.75
C208	C	1.13153	0.46957	0.75
C209	C	1.11641	0.43928	0.75
C210	C	1.13132	0.42401	0.75
C211	C	1.16155	0.43912	0.75
C212	C	1.17687	0.46951	0.75
C213	C	1.16176	0.4845	0.75
N214	N	1.16155	0.39385	0.75
N215	N	0.99548	0.55991	0.75
C216	C	0.67804	0.46901	0.75
C217	C	0.70828	0.4843	0.75
C218	C	0.72339	0.51459	0.75
C219	C	0.70807	0.52947	0.75
C220	C	0.67783	0.51436	0.75
C221	C	0.66293	0.48418	0.75
C222	C	0.66293	0.43872	0.75
N223	N	0.63269	0.42361	0.75
C224	C	0.61758	0.3935	0.75
O225	O	0.63269	0.46906	0.75
C226	C	0.75362	0.52971	0.75
C227	C	0.45151	0.37865	0.75
O228	O	0.57244	0.43893	0.75
C229	C	0.58735	0.37839	0.75
N230	N	0.57223	0.39337	0.75
C231	C	0.542	0.37826	0.75
C232	C	0.54221	0.42382	0.75
C233	C	0.52709	0.43899	0.75
C234	C	0.49686	0.42387	0.75
C235	C	0.48174	0.39377	0.75
C236	C	0.49686	0.3786	0.75
C237	C	0.52709	0.39353	0.75

N238	N	0.76874	0.55999	0.75
N239	N	0.4364	0.39382	0.75
N240	N	1.16155	1.11894	0.75