Electronic Supplementary Information (ESI)

Phenoxazine as a high-voltage p-type redox center for organic battery cathode materials: small structural reorganization for faster charging and narrow operating voltage

Kyunam Lee,[a] Illia E. Serdiuk,[ab] Giyun Kwon,[c] Dong Joo Min,[a] Kisuk Kang,[cde] Soo Young Park,*[a] and Ji Eon Kwon*[af]

[a]Center for Supramolecular Optoelectronic Materials (CSOM), Department of Materials Science and Engineering, Research Institute of Advanced Materials (RIAM), Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea

[b]Faculty of Mathematics, Physics and Informatics, University of Gdańsk, Wita Stwosza 57, 80-308 Gdańsk, Poland

[c]Department of Materials Science and Engineering, Research Institute of Advanced Materials (RIAM), Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Republic of Korea

[d]Institute of Engineering Research, College of Engineering, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Republic of Korea

[e]Center for Nanoparticle Research, Institute of Basic Science, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Republic of Korea

[f]Current Address: Center for Functional Composite Materials, Institute of Advanced Composite Materials, Korea Institute of Science and Technology, 92 Chudong-ro, Wanju-gun, Jeonbuk 55324, Republic of Korea

*e-mail: jekwon@kist.re.kr (JEK), parksy@snu.ac.kr (SYP)

Contents

1 Synthesis and characterization data

1.1 Synthesis

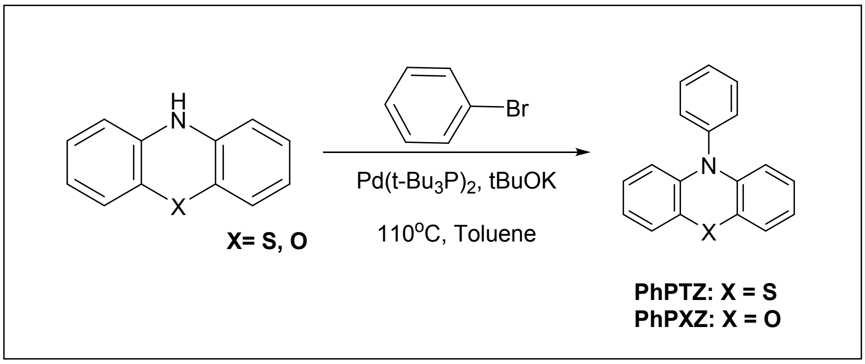


Fig. S1 Synthetic routes of PhPTZ and PhPXZ

1.1.1 Synthesis of 10-phenyl-10*H*-phenothiazine (PhPTZ)

PhPTZ was prepared according to the reported method with minor modifications.[1] In a flame-dried two-necked round bottom flask, 10*H*-phenothiazine (500 mg, 2.51 mmol), bromobenzene (590 mg, 3.76 mmol), potassium tert-butoxide (843 mg, 7.53 mmol), and bis(tri-tert-butylphosphine)palladium(0) (12.8 mg, 0.0250 mmol) were dissolved in freshly distilled toluene (10 mL). The solution was refluxed and stirred overnight. After cooling to room temperature, the reaction mixture was poured into water and extracted three times with dichloromethane. The organic layer was dried over anhydrous $MgSO_4$ and purified by flash column chromatography on silica gel with ethyl acetate/n-hexane (1:19 v/v) as an eluent to give a colorless powder. Yield: 92% (598 mg), NMR signals fully matched those previously reported.[1]

1.1.2 Synthesis of 10-phenyl-10*H*-phenoxazine (PhPXZ)

PhPXZ was prepared according to the reported method with minor modifications.[2] In a flame-dried two-necked round bottom flask, 10*H*-phenoxazine (500 mg, 2.73 mmol), bromobenzene

(643 mg, 4.09 mmol), potassium tert-butoxide (918 mg, 8.19 mmol), and bis(tri-tert-butylphosphine)palladium(0) (14 mg, 0.0273 mmol) were dissolved in freshly distilled toluene (10 mL). The solution was refluxed and stirred overnight. After cooling to room temperature, the reaction mixture was poured into water and extracted three times with dichloromethane. The organic layer was dried over anhydrous $MgSO_4$ and purified by flash column chromatography on silica gel with ethyl acetate/n-hexane (1:9 v/v) as an eluent to give a white powder. Yield: 77% (545 mg), NMR signals fully matched those previously reported.[2]

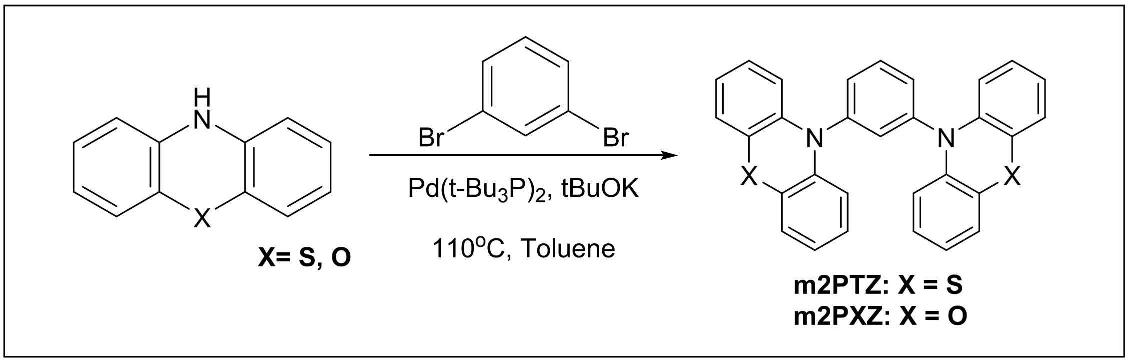


Fig. S2 Synthetic routes of m2PTZ and m2PXZ

1.1.3 Synthesis of 1,3-di(10*H*-phenothiazin-10-yl)benzene (m2PTZ)

In a flame-dried two-necked round bottom flask, 1,3-dibromobenzene (500 mg, 2.12 mmol), 10*H*-phenothiazine (1.06 g, 5.30 mmol), potassium tert-butoxide (1.19 g, 10.6 mmol), and bis(tri-tert-butylphosphine)palladium(0) (21.7 mg, 0.0424 mmol) were dissolved in freshly distilled toluene (20 mL). The solution was refluxed and stirred overnight. After cooling to room temperature, the reaction mixture was poured into water and extracted three times with dichloromethane. The organic layer was dried over anhydrous $MgSO_4$ and purified by column chromatography on silica gel with ethyl acetate/n-hexane (1:19 v/v) as an eluent. Recrystallization from methanol/chloroform (1:1 v/v) afforded a white powder. Yield: 82%

(0.82 g), ^{1}H-NMR (300 MHz, $CDCl_3$) δ(ppm): 7.72 (t, J = 8.1 Hz, 1H), 7.42 (d, J = 8.1 Hz, 2H), 7.35 (s, 1H), 7.10 (d, *J* = 7.5 Hz, 4H), 6.97-6.85 (m, 8H), 6.46 (d, *J* = 7.8 Hz, 4H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ(ppm): 144.21, 143.92 132.39, 129.55, 128.12, 127.38, 127.19, 123.35, 122.56, 117.63; HRMS (FAB+): calcd. for $C_{30}H_{20}N_2S_2$ (M^+), 472.1068; found, 472.1064

1.1.4 Synthesis of 1,3-di(10*H*-phenoxazin-10-yl)benzene (m2PXZ)

In a flame-dried two-necked round bottom flask, 1,3-dibromobenzene (500 mg, 2.12 mmol), 10*H*-phenoxazine (0.97 g, 5.30 mmol), potassium tert-butoxide (1.19 g, 10.6 mmol), and bis(tri-tert-butylphosphine)palladium(0) (21.7 mg, 0.0424 mmol) were dissolved in freshly distilled toluene (20 mL). The solution was refluxed and stirred overnight. After cooling to room temperature, the reaction mixture was poured into water and extracted three times with dichloromethane. The organic layer was dried over anhydrous $MgSO_4$ and purified by column chromatography on silica gel with ethyl acetate/n-hexane (1:19 v/v) as an eluent. Recrystallization from methanol/chloroform (1:1 v/v) afforded a white powder. Yield: 72% (0.68 g), ^{1}H-NMR (300 MHz, $CDCl_3$) δ(ppm): 7.82 (t, J = 7.8 Hz, 1H), 7.50 (d, J = 7.8 Hz, 2H), 7.41 (s, 1H), 6.71-6.61 (m, 12H), 6.01 (d, *J* = 6.9 Hz, 4H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ(ppm): 144.16, 142.01, 134.15, 133.89, 133.69, 131.48, 123.52, 121.92, 115.90, 113.30; HRMS (FAB+): calcd. for $C_{30}H_{20}N_2O_2$ (M^+), 440.1525; found, 440.1517

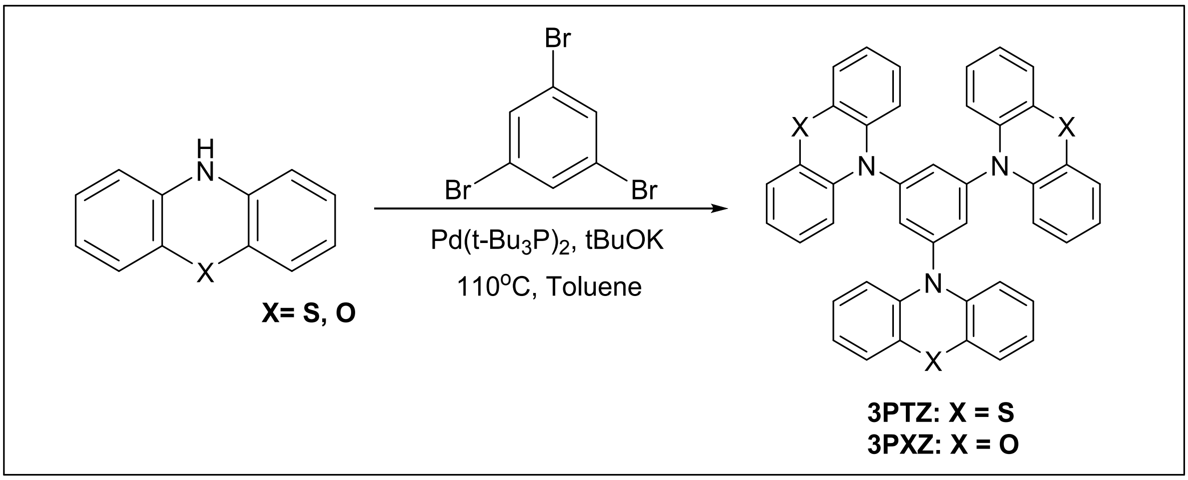


Fig. S3 Synthetic routes of 3PTZ and 3PXZ

1.1.5 Synthesis of 1,3,5-tri(10*H*-phenothiazin-10-yl)benzene (3PTZ)

In a flame-dried two-necked round bottom flask, 1,3,5-tribromobenzene (1.00 g, 3.18 mmol), 10*H*-phenothiazine (2.22 g, 11.1 mmol), potassium tert-butoxide (1.78 g, 15.9 mmol), and bis(tri-tert-butylphosphine)palladium(0) (48.7 mg, 0.0953 mmol) were dissolved in freshly distilled toluene (30 mL). The solution was refluxed and stirred overnight. After cooling to room temperature, the reaction mixture was poured into water and extracted three times with dichloromethane. The organic layer was dried over anhydrous $MgSO_4$ and purified by column chromatography on silica gel with ethyl acetate/n-hexane (1:9 v/v) as an eluent. Recrystallization from methanol/chloroform (1:3 v/v) afforded a whitish gray crystal. Yield: 80% (1.70 g), ^{1}H-NMR (300 MHz, DMSO) δ(ppm): 7.26 (d, J = 7.5 Hz, 6H), 7.15 (t, J = 7.8 Hz, 6H), 7.04 (t, J = 7.5 Hz, 6H), 6.95 (s, 3H), 6.80 (d, *J* = 8.1 Hz, 6H); ^{13}C-NMR (125 MHz, DMSO) δ(ppm): 145.83, 142.23, 127.63, 127.60, 124.66, 124.38, 120.11, 117.29; HRMS (FAB+): calcd. for $C_{42}H_{27}N_3S_3$ (M^+), 669.1367; found, 669.1367

1.1.6 Synthesis of 1,3,5-tri(10*H*-phenoxazin-10-yl)benzene (3PXZ)

In a flame-dried two-necked round bottom flask, 1,3,5-tribromobenzene (1.00 g, 3.18 mmol), 10*H*-phenoxazine (2.04 g, 11.1 mmol), potassium tert-butoxide (1.78 g, 15.9 mmol), and bis(tri-tert-butylphosphine)palladium(0) (48.7 mg, 0.0953 mmol) were dissolved in freshly distilled toluene (30 mL). The solution was refluxed and stirred overnight. After cooling to room temperature, the reaction mixture was poured into water and extracted three times with dichloromethane. The organic layer was dried over anhydrous $MgSO_4$ and purified by column chromatography on silica gel with ethyl acetate/n-hexane (1:9 v/v) as an eluent. Recrystallization from methanol/chloroform (1:1 v/v) afforded a yellow crystal. Yield: 75% (1.5 g), ^{1}H-NMR (300 MHz, $CDCl_3$) δ(ppm): 7.54 (s, 3H), 6.72-6.69 (m, 18H), 6.11 (d, J = 4.8 Hz, 6H); ^{13}C-NMR (125 MHz, DMSO) δ(ppm): 143.92, 143.19 133.99, 133.43, 123.89, 121.88, 115.48, 113.35; HRMS (FAB+): calcd. for $C_{42}H_{27}N_3O_3$ (M^+), 621.2057; found, 621.2052

1.2 Characterization data

1.2.1 ^{1}H-NMR & ^{13}C-NMR spectra

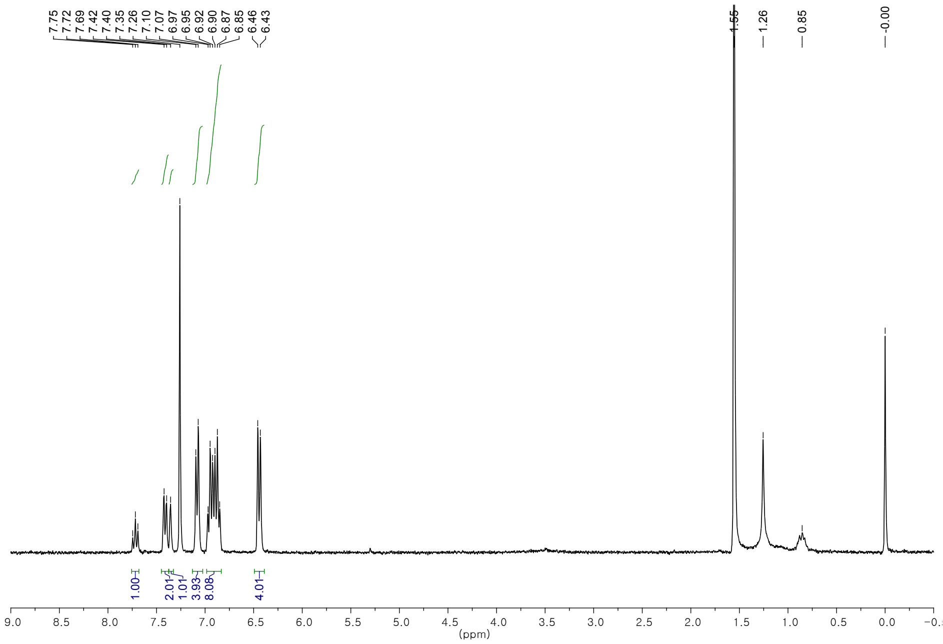


Fig. S4 300 MHz ^{1}H-NMR spectrum of **m2PTZ** in CDCl3

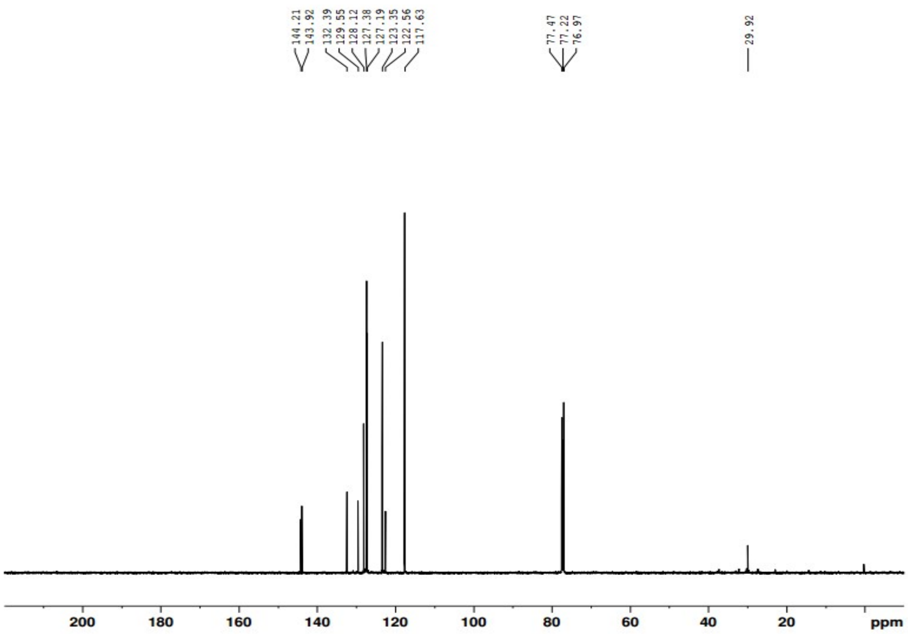


Fig. S5 125 MHz ^{13}C-NMR spectrum of **m2PTZ** in CDCl3

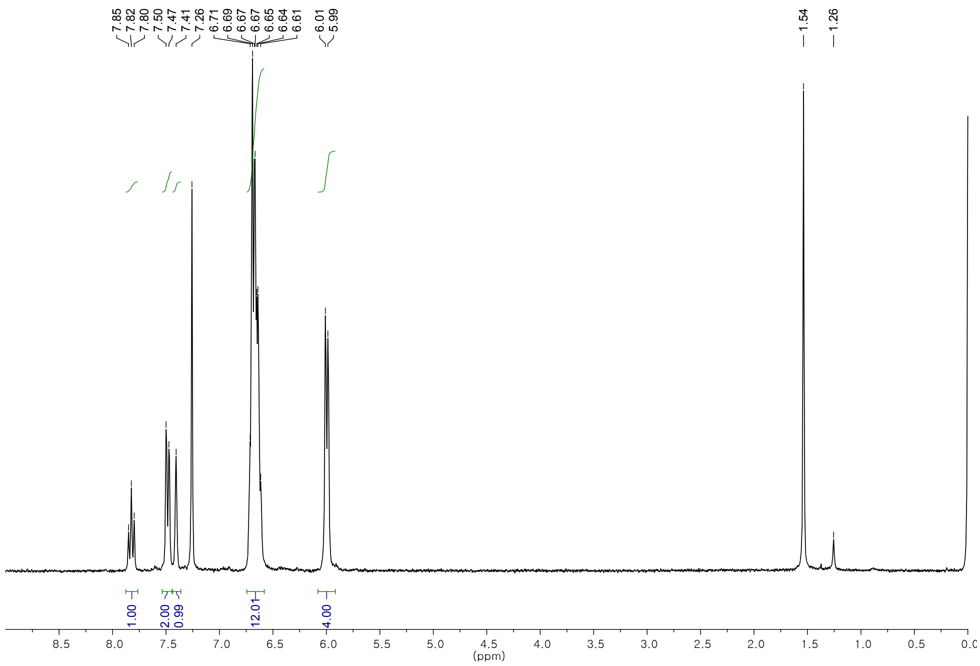


Fig. S6 300 MHz ^{1}H-NMR spectrum of **m2PXZ** in CDCl3

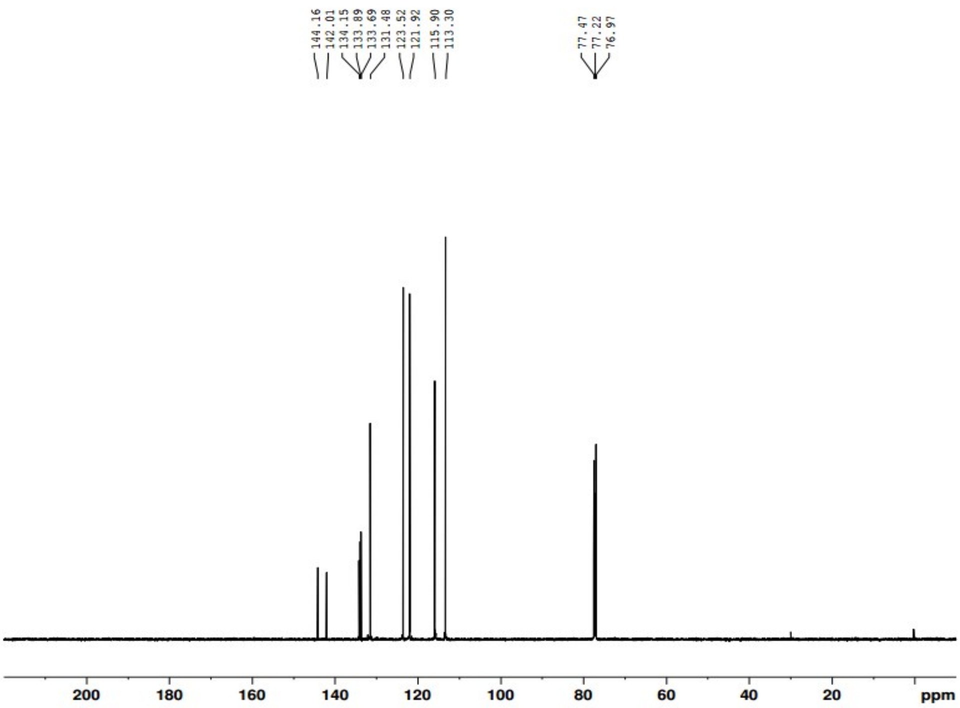


Fig. S7 125 MHz ^{13}C-NMR spectrum of **m2PXZ** in CDCl3

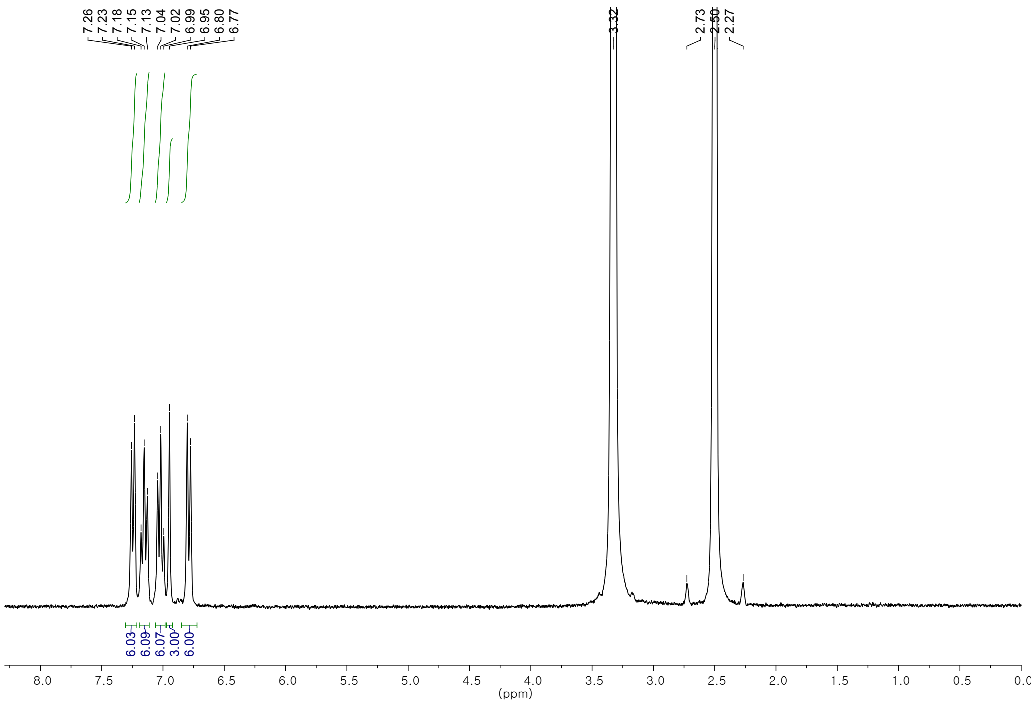


Fig. S8 300 MHz ^{1}H-NMR spectrum of **3PTZ** in DMSO

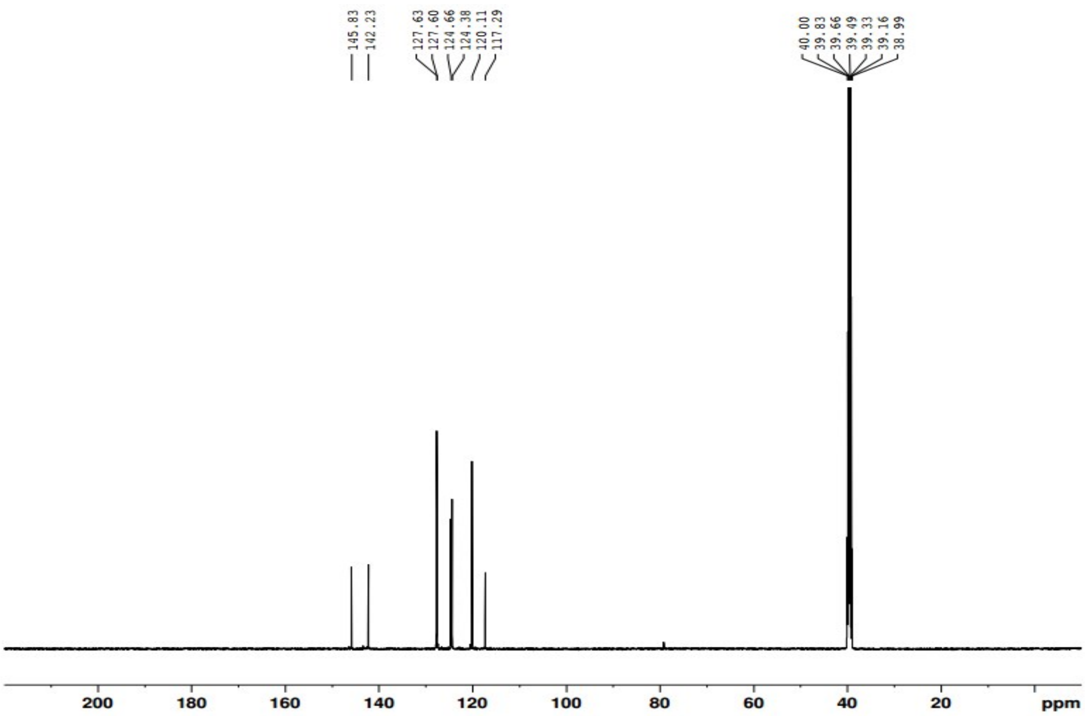


Fig. S9 125 MHz ^{13}C-NMR spectrum of **3PTZ** in DMSO

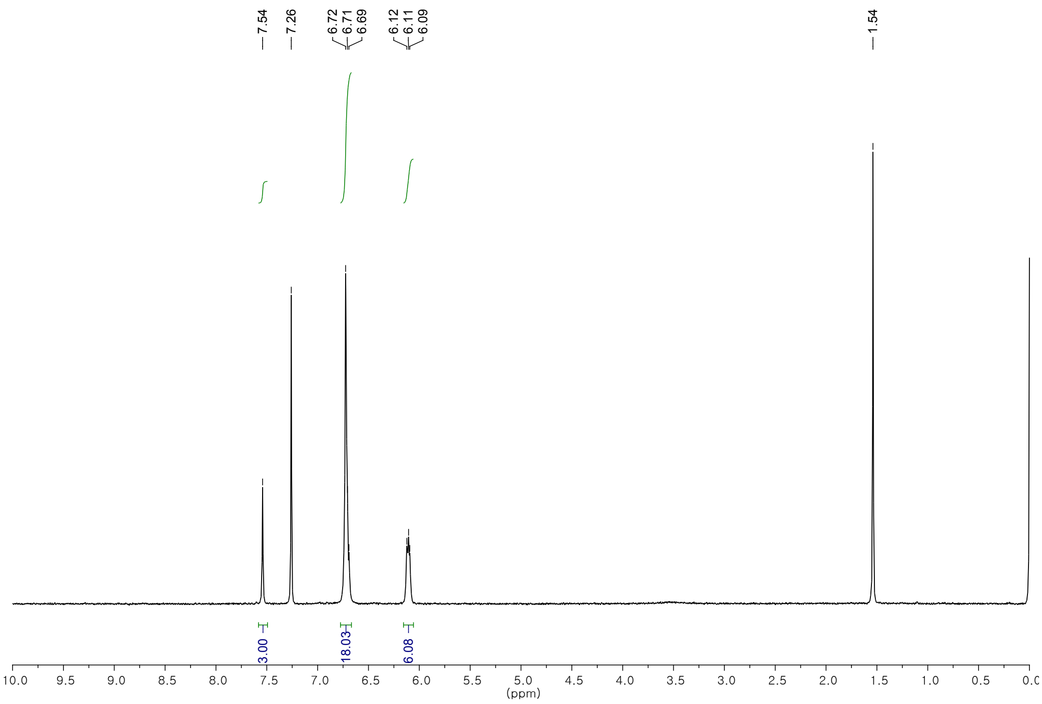


Fig. S10 300 MHz ^{1}H-NMR spectrum of **3PXZ** in $CDCl_3$

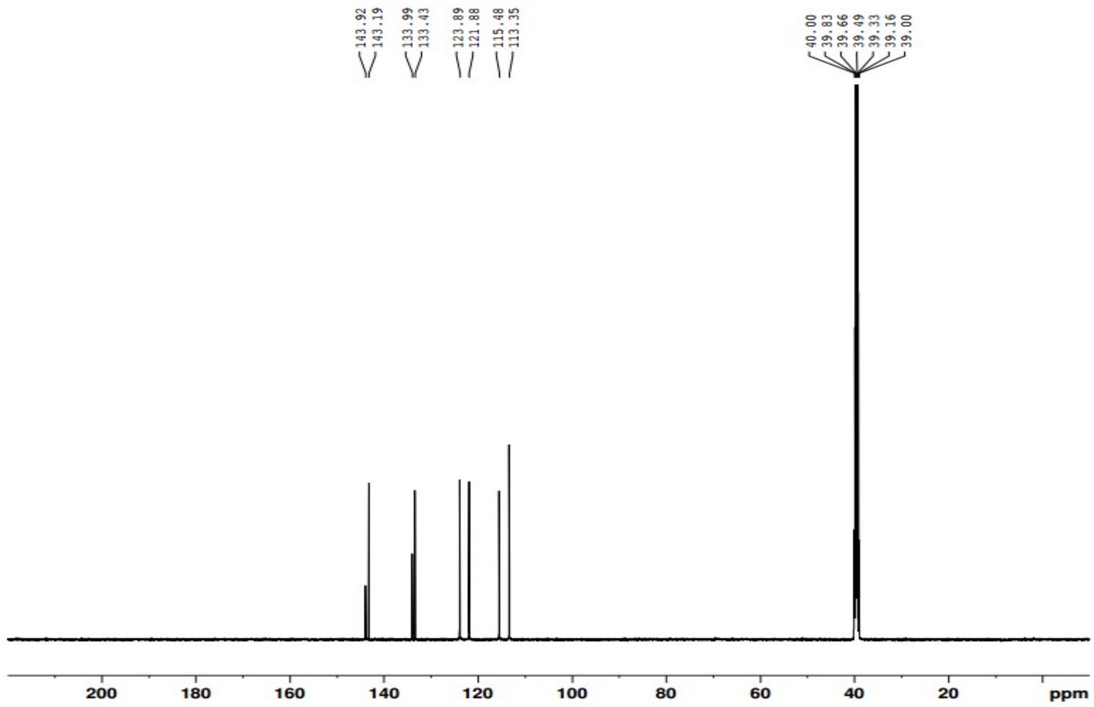


Fig. S11 125 MHz ^{13}C-NMR spectrum of **3PXZ** in DMSO

2. Investigation of PTZ and PXZ derivatives

2.1 Rotating disk electrode test of PhPTZ and PhPXZ

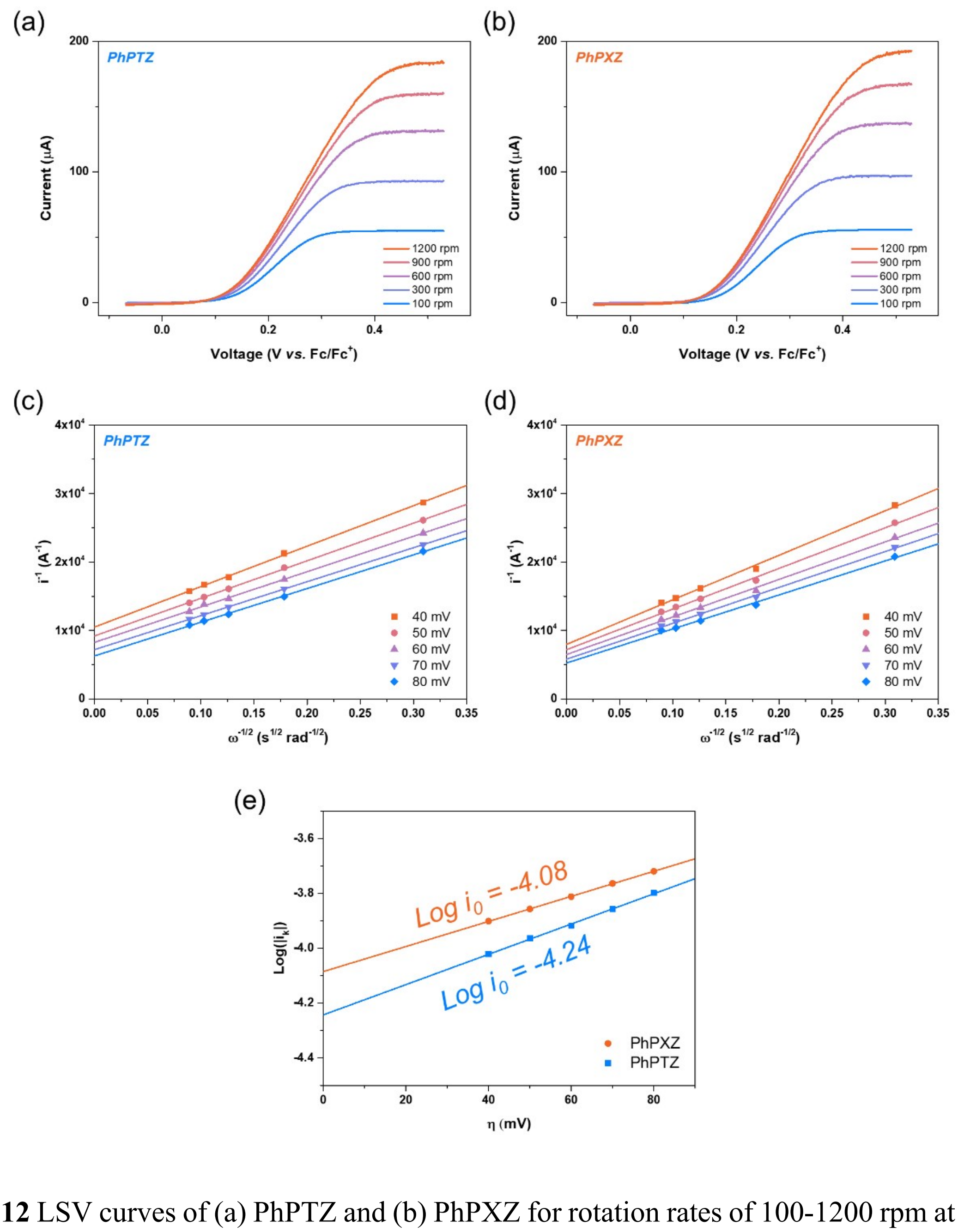


Fig. S12 LSV curves of (a) PhPTZ and (b) PhPXZ for rotation rates of 100-1200 rpm at a scan rate of 5 mV s^{-1}. Linearly fitted Koutecký-Levich plots of (c) PhPTZ and (d) PhPXZ at various overpotentials. (e) Linearly fitted plots of logarithm of kinetics-controlled current (log i_k) as a function of overpotential (η).

2.2 Galvanostatic charge/discharge test of PhPTZ and PhPXZ

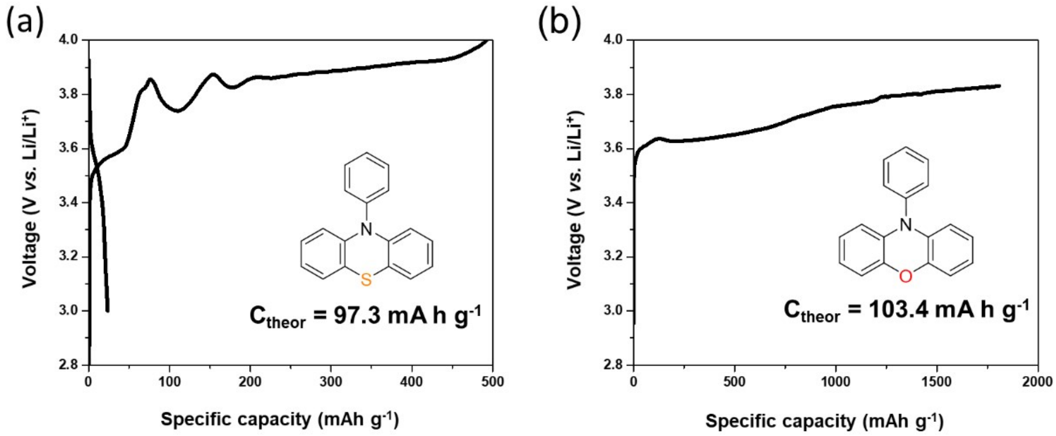


Fig. S13 The charge/discharge profiles of the first cycle for (a) PhPTZ and (b) PhPXZ electrode at 1 C rate. 2 M LiTFSI with 1 wt% $LiNO_3$ in DOL/DME (1:1 v/v) was used as an electrolyte. The C rate of each material was calculated by its theoretical capacity, which corresponds to 97.3 mA g^{-1} and 103.4 mA g^{-1} for PhPTZ and PhPXZ, respectively.

2.3 Optimized molecular structures of 3PTZ and 3PXZ

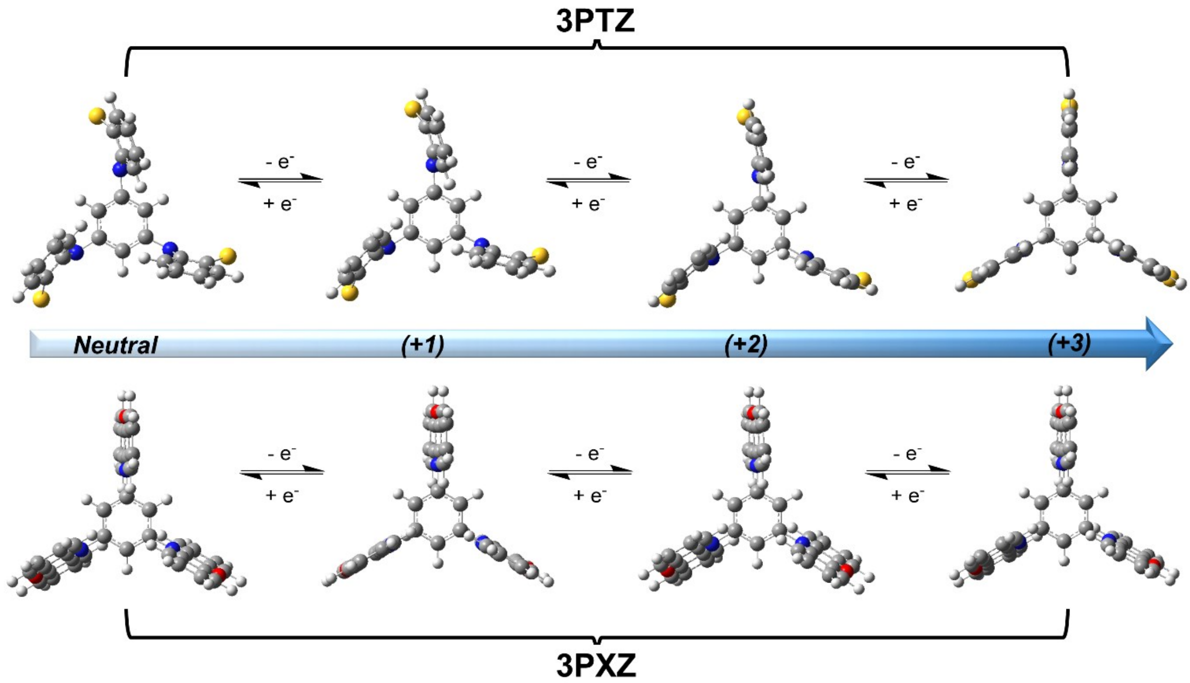


Fig. S14 The front views of the optimized molecular structures of 3PTZ and 3PXZ obtained by DFT calculation. In each oxidation state, all three active groups (*e.g.*, PTZ or PXZ) in the molecule had same geometry.

2.4 Cyclic voltammograms of 3PXZ and 3PTZ

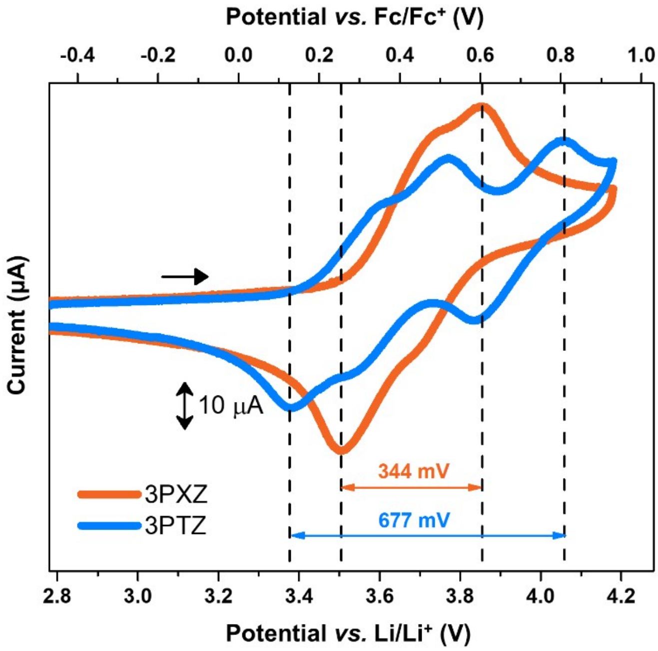


Fig. S15 The peak separation between the anodic peak of the last reaction and the cathodic peak of the first reaction on cyclic voltammograms of 3PXZ and 3PTZ. Cyclic voltammograms were obtained in CH_2Cl_2 solution (c = 1mM) with 0.1 M n-Bu_4NPF_6 supporting electrolyte at a scan rate of 100 mV s^{-1}.

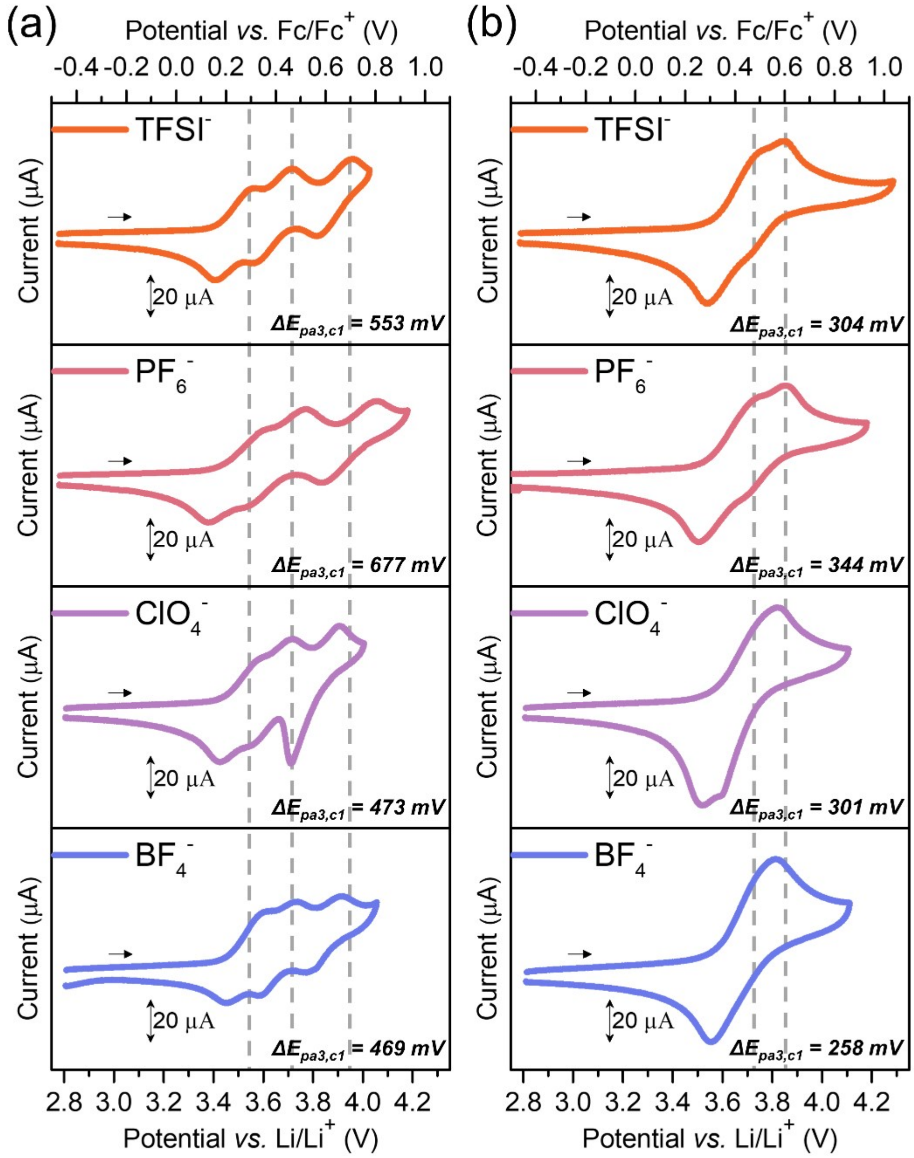


Fig. S16 CVs of (a) 3PTZ, and (b) 3PXZ in 0.1 M $TBABF_4$, $TBAClO_4$, $TBAPF_6$, and TBATFSI in CH_2Cl_2.

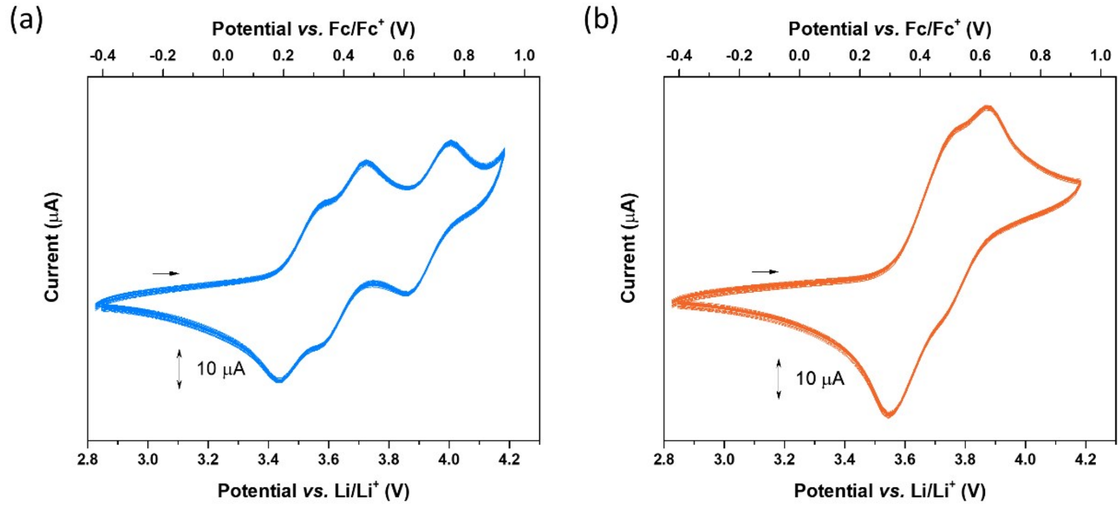


Fig. S17 Cyclic voltammograms of (a) 3PTZ and (b) 3PXZ for 50 cycles in CH_2Cl_2 solution (c = 1 mM) with 0.1 M TBAPF6 supporting electrolyte at a scan rate of 100 mV s^{-1}.

2.5 Theoretical calculation for oxidation process

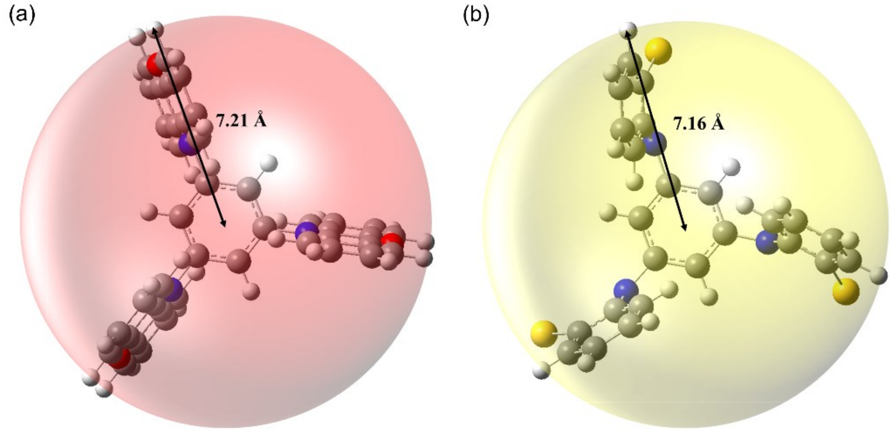


Fig. S18 Molecular skeleton and radius of (a) 3PXZ and (b) 3PTZ. The radius corresponds to the distance between centroid of the molecule and the farthest atom from the centroid.

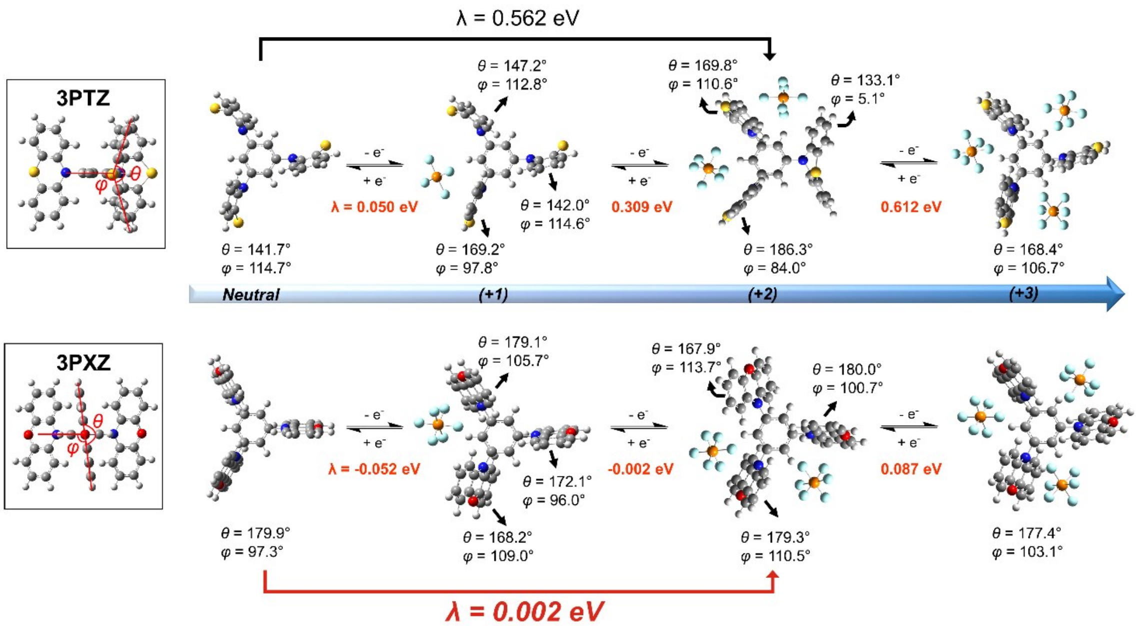


Fig. S19 The optimized structures of 3PTZ and 3PXZ in the four different oxidation states (*i.e.*, the neutral, +1, +2, and +3 states) with PF_6^- anions obtained by DFT calculation (B3LYP functional and 6-311G+(d,p) basis set). The reorganization energy (λ) in eV for each oxidation step were determined using results of single-point energy calculation of the molecules at each optimized organic skeleton without anions. See Materials and Methods section for the calculation details.

2.6 SEM images for optimization of electrode fabrication processes

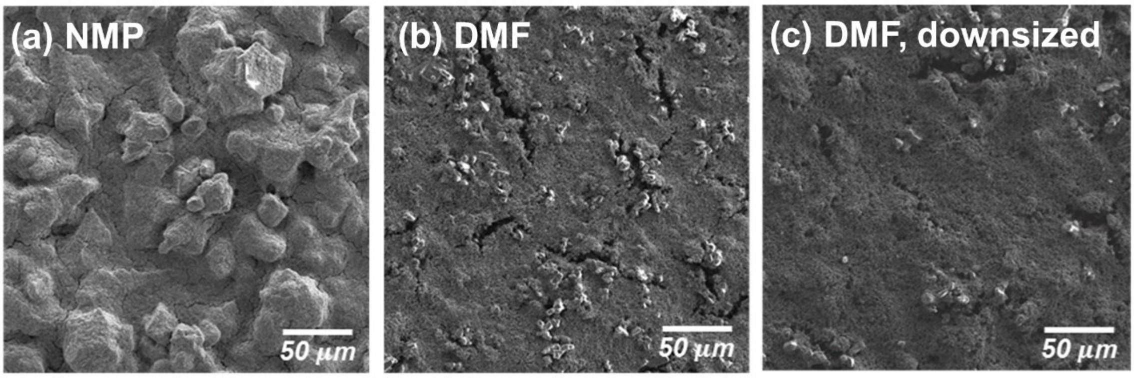


Fig. S20 SEM images of 3PXZ electrodes prepared by various conditions: (a) NMP and (b) DMF was used as the slurry-making solvent. (c) DMF was used as the slurry-making solvent, and the downsized particle of 3PXZ by the antisolvent precipitation process was used.

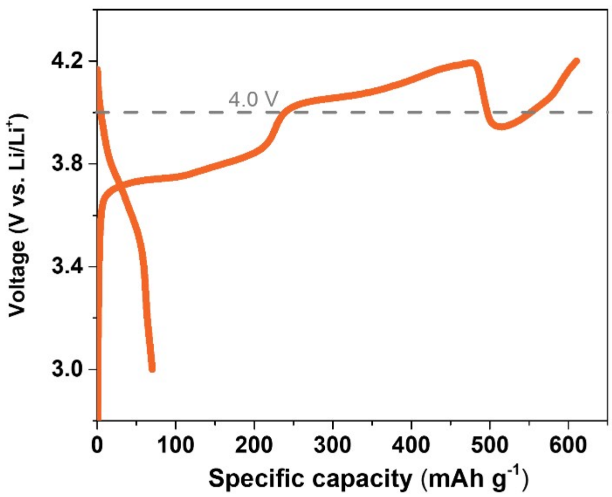


Fig. S21 The galvanostatic charge/discharge profile of 3PXZ in voltage range 3.0 V – 4.2 V at current rate of 1C.

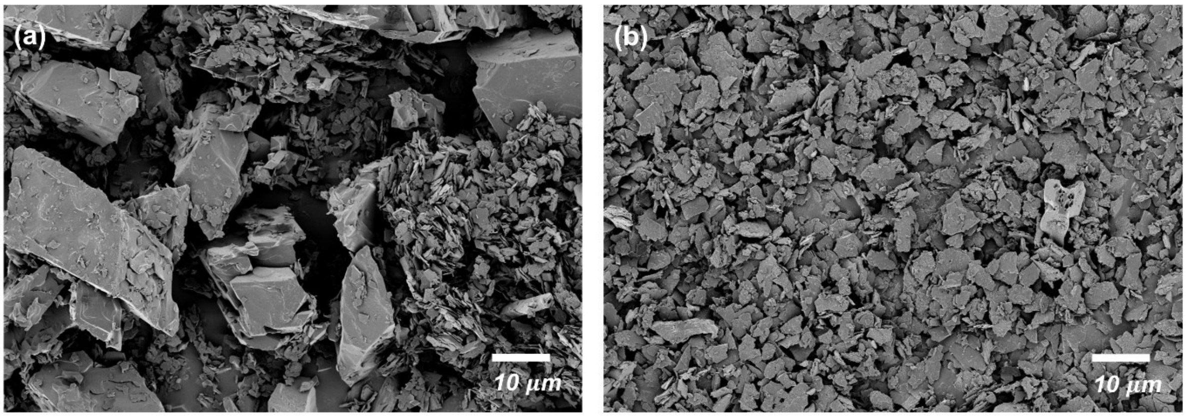


Fig. S22 SEM images of (a) the pristine 3PXZ powders and (b) the downsized 3PXZ powders after the antisolvent precipitation process. The particle size of 3PXZ powders was obviously reduced after the antisolvent precipitation process.

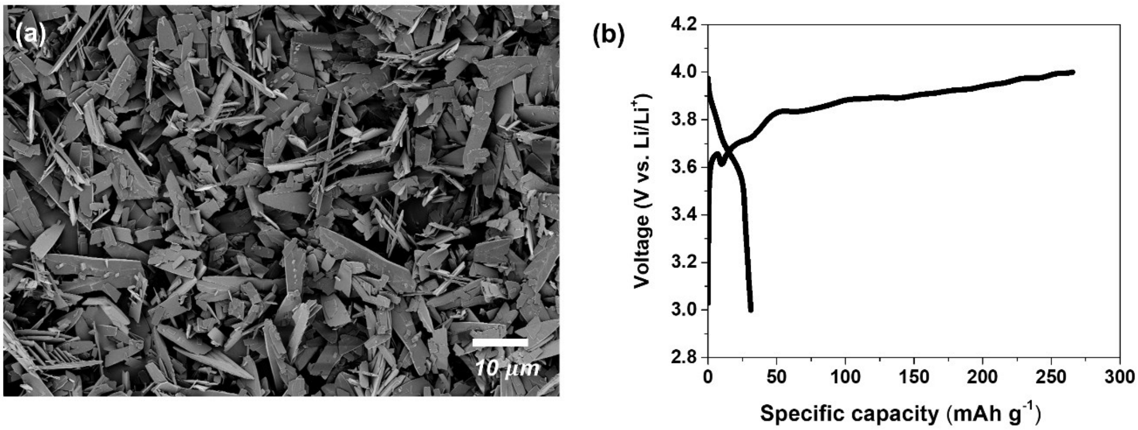


Fig. S23 (a) SEM image of the downsized 3PTZ particles after the antisolvent precipitation process. (b) Galvanostatic charge/discharge profile (1st cycle) of the electrode fabricated with downsized 3PTZ at a current rate of 1 C.

2.7 Electrochemical performance of 3PTZ and 3PXZ electrodes

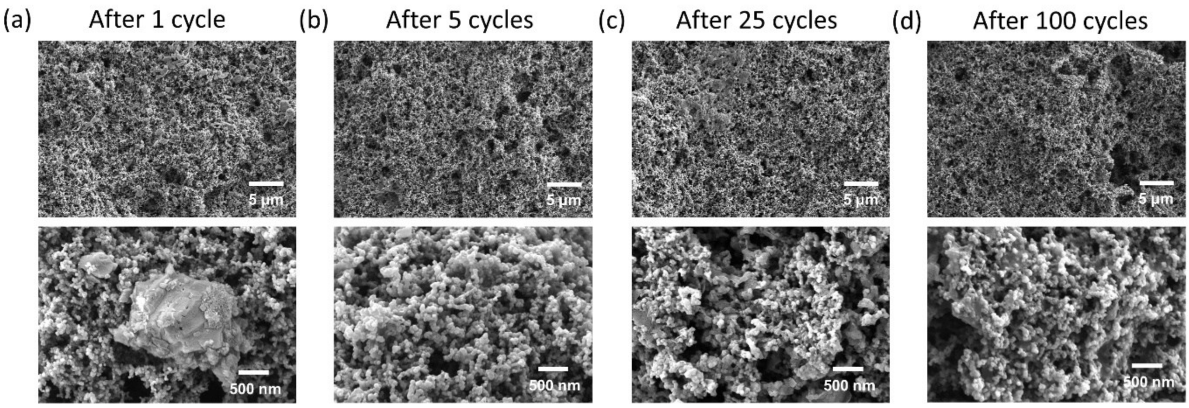


Fig. S24 SEM images of the surface of 3PXZ electrodes after (a) 1 (b) 5 (c) 25 (d) 100 charge/discharge cycle(s).

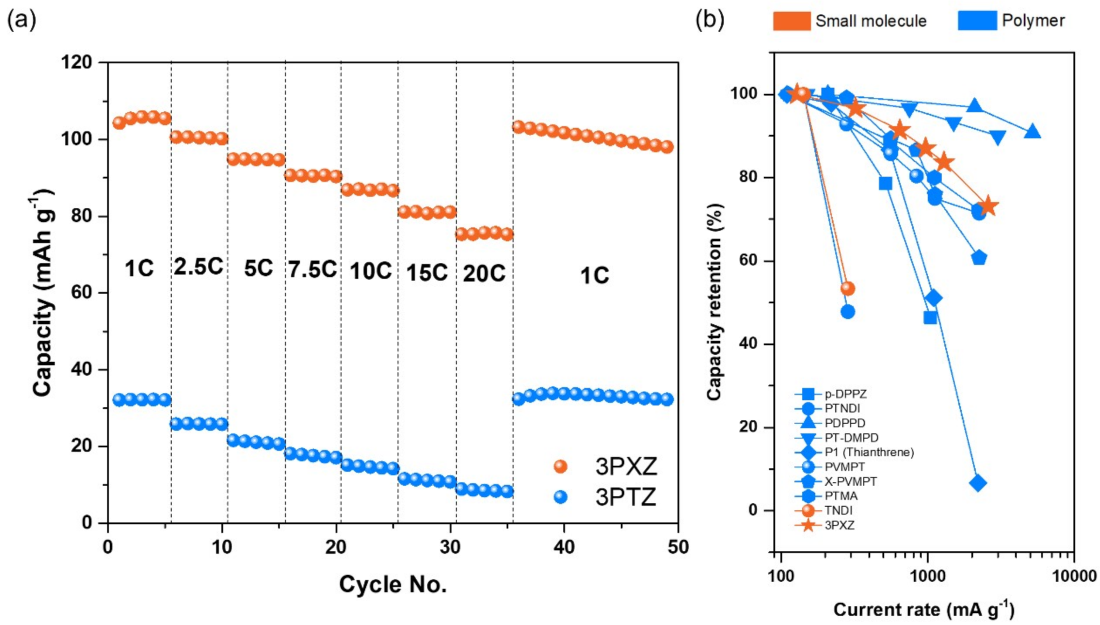


Fig. S25 (a) Rate capability test of 3PTZ and 3PXZ electrodes at various C rate. Five initial activation cycles at 1C rate were conducted for the both electrodes before measurements. (b) Comparison of rate capability of the reported organic p-type cathode materials: small molecules (orange color) and polymers (blue color). Capacities at various current rates were normalized by their capacities at 1C rate and represented as capacity retention (%). See Table S2 for the detailed data used in this graph.

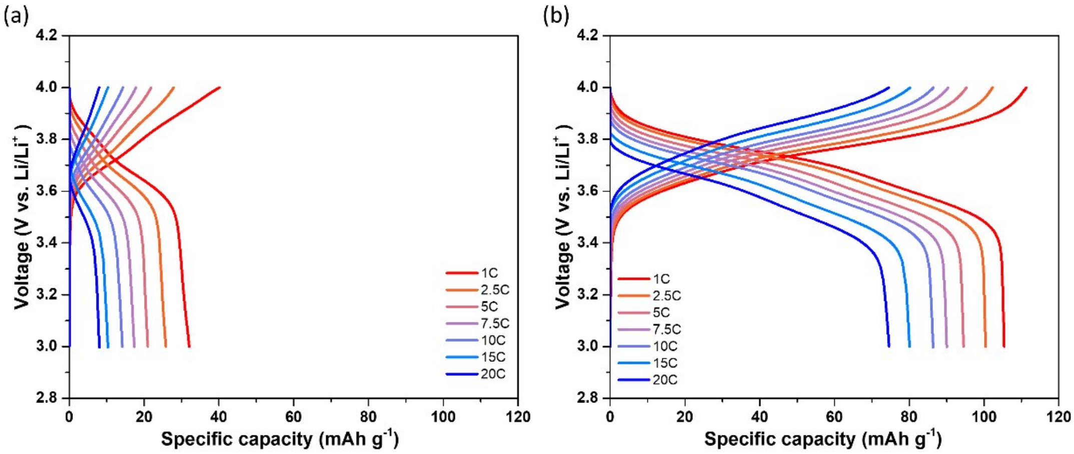


Fig. S26 Electrochemical profiles of (a) 3PTZ and (b) 3PXZ, under different C-rates.

2.8 Ex-situ Analyses

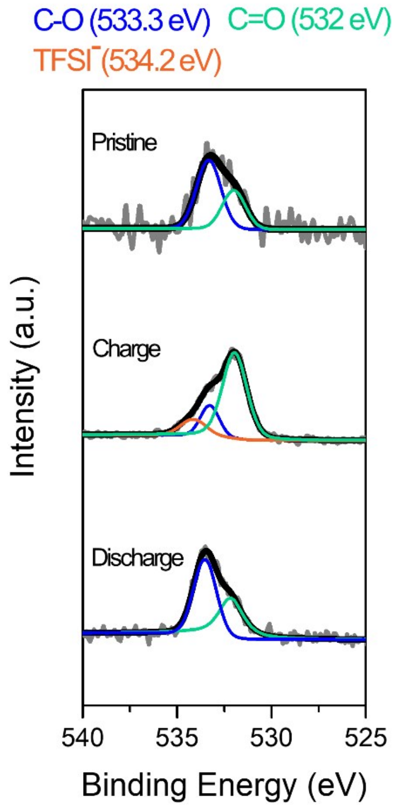


Fig. S27 Ex-situ O 1s XPS spectra of 3PXZ electrodes in the pristine, charged, and discharged states.

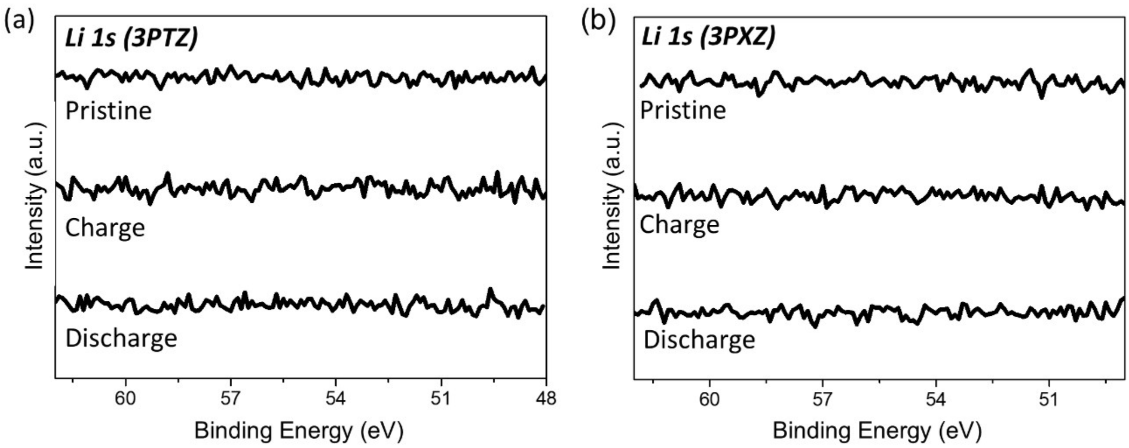


Fig. S28 Li 1s spectra of ex-situ XPS measurements for (a) 3PTZ and (b) 3PXZ electrodes. No signals appeared for all ex-situ samples, which indicates Li ion-free redox reactions and complete removal of LiTFSI electrolyte by washing the ex-situ samples.

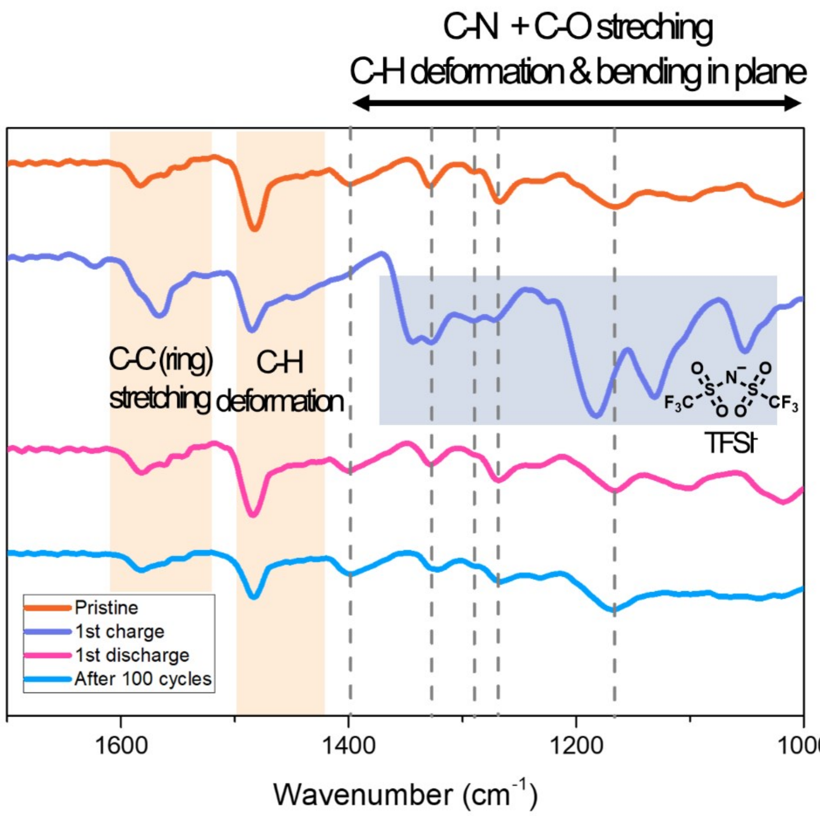


Fig. S29 FT-IR measurements of 3PXZ ex-situ electrodes.

Table S1. $TFSI^-$ peak assignments for the FT-IR spectra.[3]

Wavenumber (cm^{-1})	Vibrational mode
1051	Asymmetric S–N–S stretching mode of $TFSI^-$
1182	Asymmetric stretching mode of CF3 of $TFSI^-$
1131, 1326	C–SO_2–N bonding mode of $TFSI^-$
1345	Asymmetric SO_2 stretching mode of $TFSI^-$

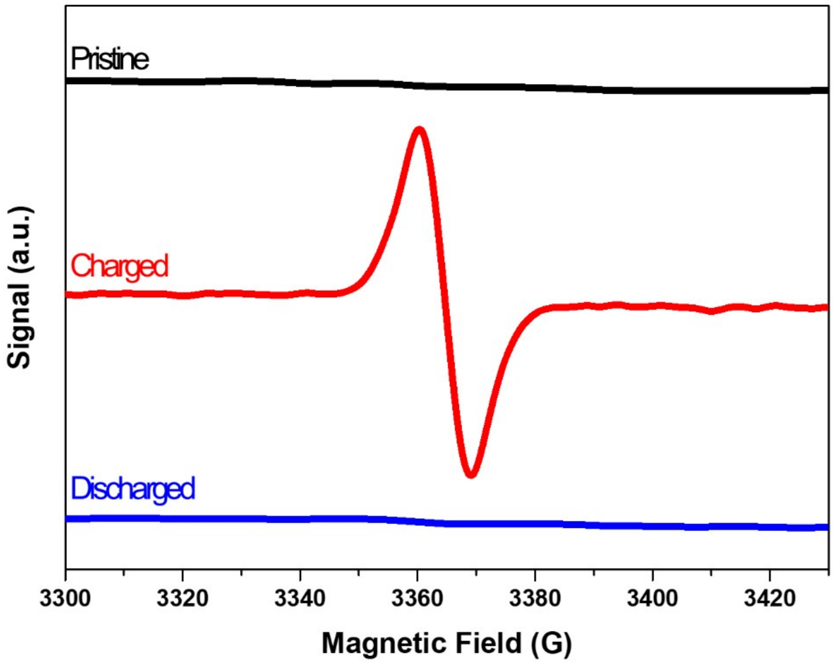


Fig. S30 Ex-situ electron spin resonance (ESR) spectroscopy measurements of 3PXZ electrodes. Only charged electrode showed ESR signal with g = 2.0030, which indicates formation of radical cations after oxidation.

2.9 CMK-3 nanocomposites

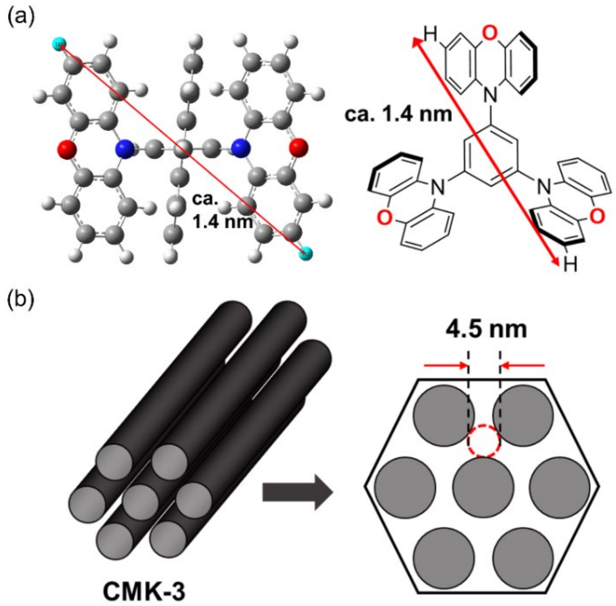


Fig. S31 (a) The maximum dimension of 3PXZ estimated by Gaussview software using the optimized structure. (b) Schematic structure of CMK-3 and its pore size.

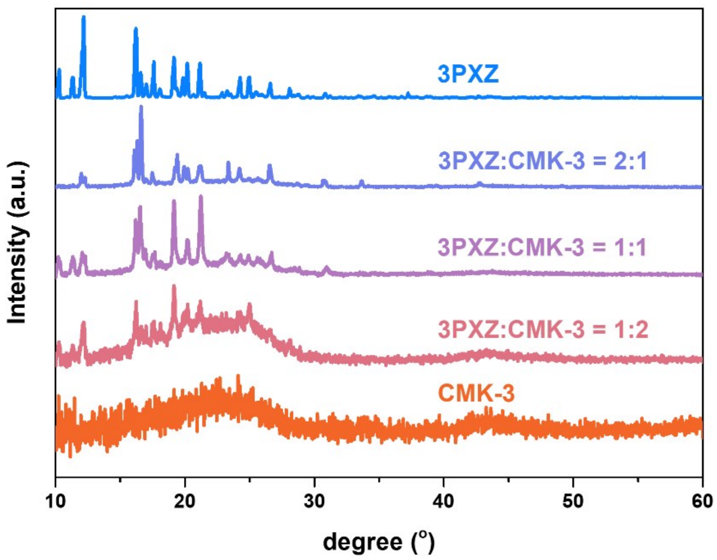


Fig. S32 PXRD spectra of the pristine 3PXZ, 3PXZ@CMK-3 composites with different mixing ratio, and the pristine CMK-3. The slightly different PXRD peaks observed in the 2:1 sample is most likely attributed to the occurrence of fast recrystallization from the supersaturated solution leading to formation of somewhat different crystal structure of 3PXZ from the other samples.

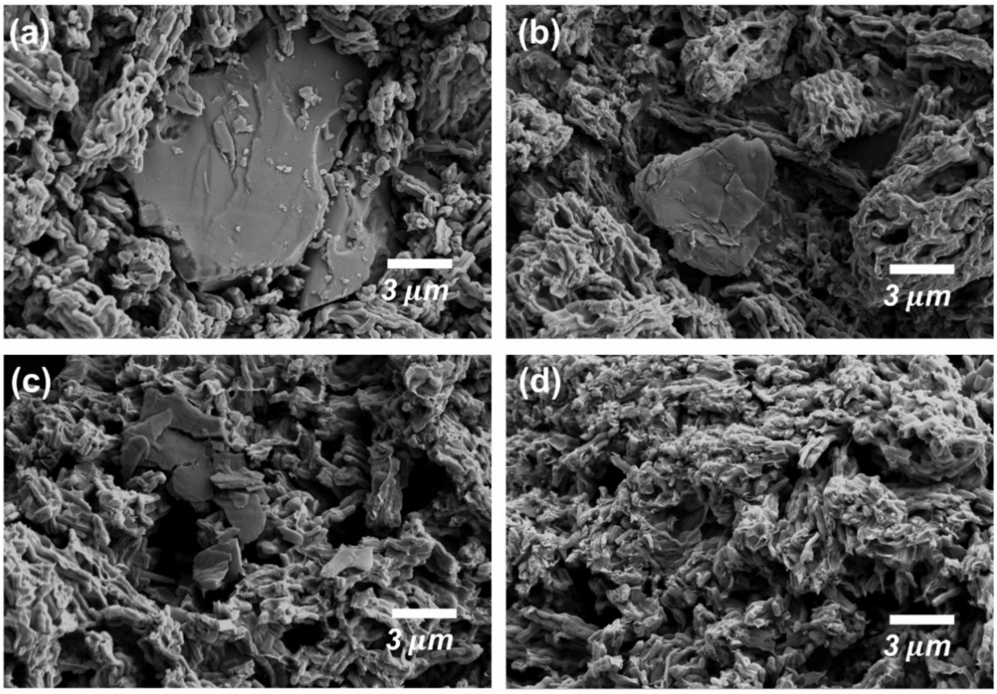


Fig. S33 SEM images of 3PXZ@CMK-3 composites with different mixing ratio: 3PXZ: CMK-3 was (a) 2:1, (b) 1:1, and (c) 1:2 in weight. (d) An SEM image of the pristine CMK-3.

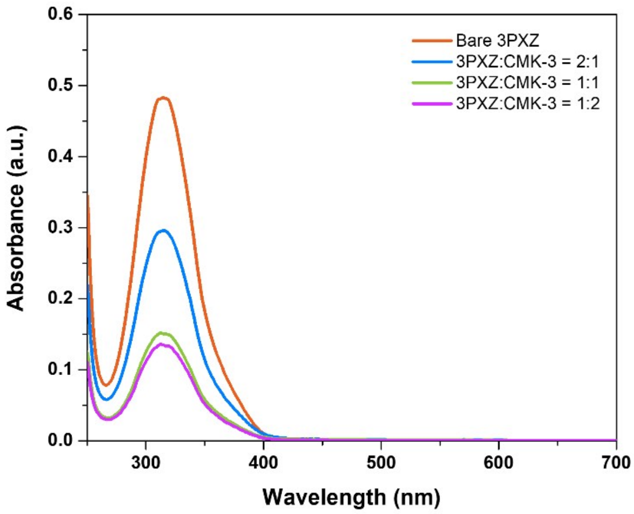


Fig. S34 UV-vis absorption spectroscopic investigations after 24 h immersion of the electrodes in the excessive amount of electrolyte. A 3 mL of 2 M LiTFSI in DOL/DME (1:1 v/v) electrolyte was used per 1 mg of 3PXZ in the electrode. After 24 h immersion, the solutions were diluted ten times for measuring absorbance.

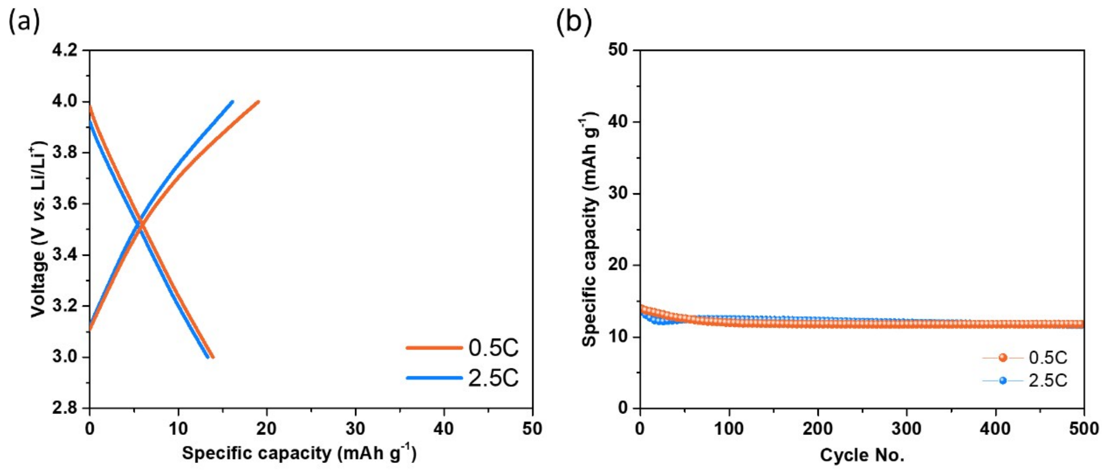


Fig. S35 (a) The charge/discharge profiles and (b) cycle data at 0.5C and 2.5C rate of the genuine CMK-3 electrode (80 wt% of CMK-3, 10 wt% of carbon black, and 10% of PVDF). Given that the weight ratio of 3PXZ:CMK-3 is 1:2 in the 3PXZ@CMK-3 composite, we evaluated the genuine CMK-3 electrode at 0.5C and 2.5C.

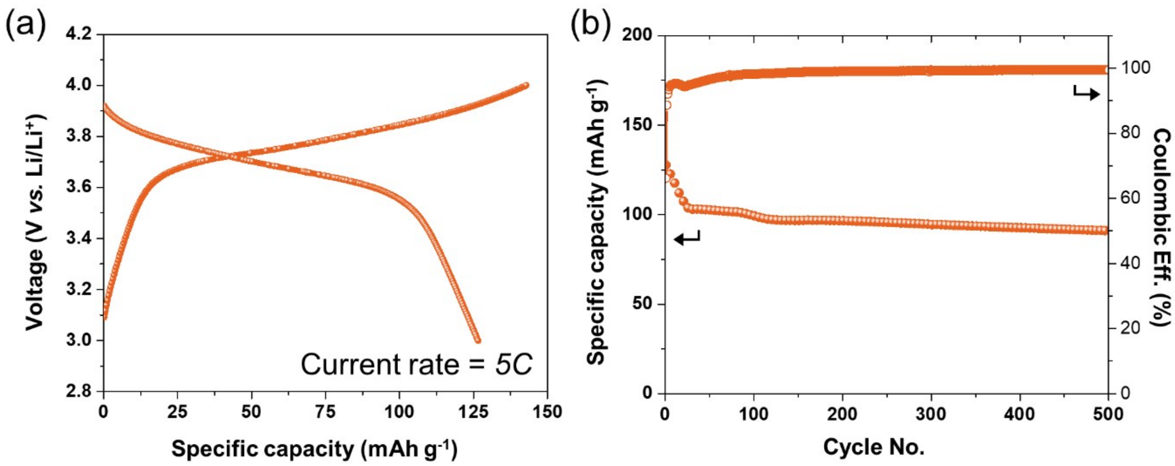


Fig. S36 (a) Representative galvanostatic charge/discharge profiles and (b) specific capacity with the corresponding coulombic efficiency obtained from the cycling stability test of 3PXZ@CMK-3 electrode at 5C, before removing the capacity contribution of CMK-3 in the composite.

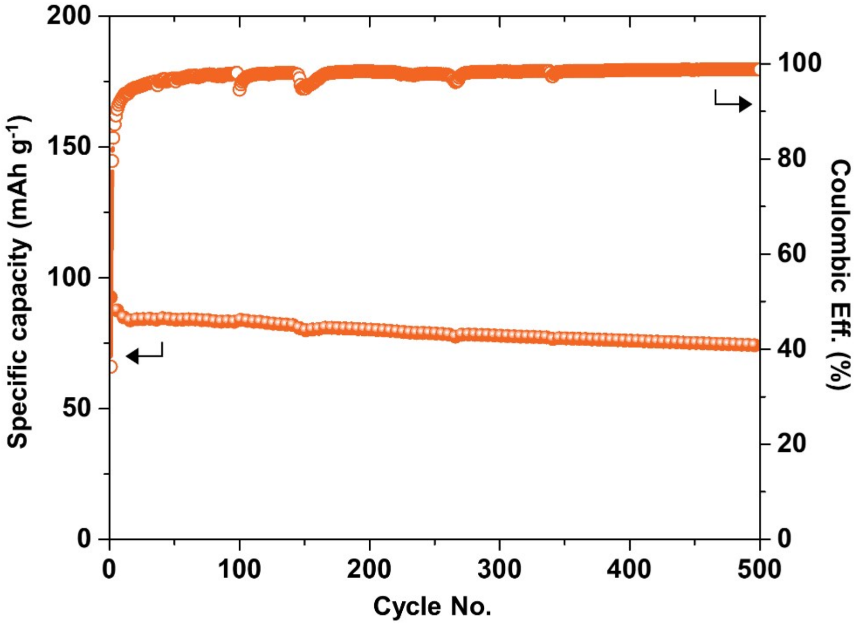


Fig. S37 Specific capacities with the corresponding coulombic efficiencies obtained from cycling stability test of 3PXZ@CMK-3 electrode at 1C rate, after removing the capacity contribution of CMK-3.

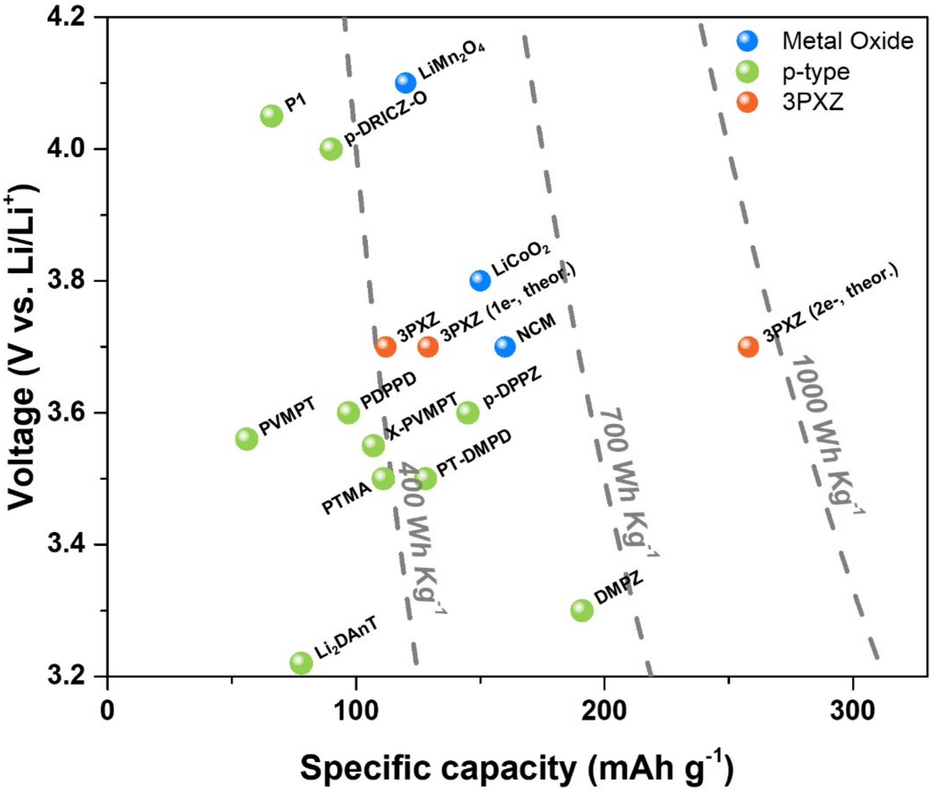
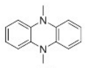
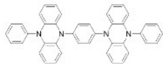
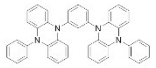
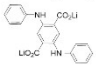
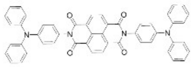
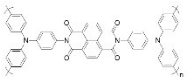
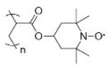
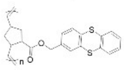
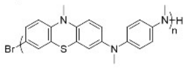
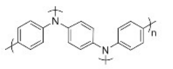
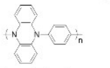
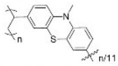
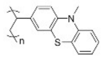
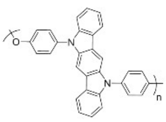


Fig. S38 Specific capacity *vs.* voltage plot of the previously reported p-type organic electrode materials, conventional inorganic materials, 3PXZ and theoretical two-electron storage specific capacity of 3PXZ. See Table S2 (ESI†) for detailed information on the reported materials used in this plot.

Table S2. Organic p-type cathode materials used in Fig. 5c and Fig S33.[4-14]

Structure	Name	Electrolyte	Average discharge voltage (V)	C_{theor} (mAh g^{-1})	C_{sp} (mAh g^{-1})	Cycling stability: Retention, cycles, current	Capacity loss per cycle[b]	Ref.
Small molecules								
	DMPZ	1 M LiTFSI in TEGDME	3.3[a]	255	191	45%, 10, 50 mA g^{-1}	8.490%	4
	pP-DPPZ	1 M LiTFSI in TEGDME	3.5[a]	182	130[a]	80%, 10, 50 mA g^{-1}	2.449%	4
	mP-DPPZ	1 M LiTFSI in TEGDME	3.5[a]	182	108[a]	62%, 10, 50 mA g^{-1}	5.173%	4
	Li_2-DAnT	1 M $LiClO_4$ in PC	3.22	148	78[a]	83%, 20, 15 mA g^{-1}	0.955%	5
	TNDI	1 M $LiPF_6$ in EC/DMC/EMC (1:1:1)	2.82	143	130[a]	62%, 100, 1C	0.477%	6
Polymers								
	PTNDI	1 M $LiPF_6$ in EC/DMC/EMC (1:1:1)	2.82	143	140	89%, 100, 1C	0.114%	6
	PTMA	1 M $LiPF_6$ in EC/DMC (1:1)	3.5	111	111	87%, 200, 1C	0.068%	7
	P1	1 M $LiPF_6$ in EC/DMC (1:1)	4.05	73	66	36%, 100, 1C	1.035%	8
	PT-DMPD	1 M $LiPF_6$ in EC/DEC (1:1)	3.5[a]	156	128	64%, 100, 1C	0.905%	9
	PDPPD	1 M $LiPF_6$ in EC/DMC (1:1)	3.6	209	97	79%, 500, 1C	0.047%	10
	p-DPPZ	1 M $LiPF_6$ in EC/DEC (1:1)	3.6[a]	209	145	90%, 500, 1C	0.022%	11
	X-PVMPT	1 M $LiPF_6$ in EC/DMC (1:1)	3.55	112	107	95%, 900, 1C	0.005%	12
	PVMPT	1 M $LiPF_6$ in EC/DMC (1:1)	3.55	112	56	100%, 1000, 1C	0%	13
	p-DRICZ-O	1 M $LiPF_6$ in EC/DMC (1:1)	4.0[a]	125	90	87%, 800, 1C	0.018%	14

[a]Estimated from corresponding electrochemical profiles

[b]Capacity loss per cycle was calculated by following equation: (N^{th} cycle capacity) = (1^{st} cycle capacity) * (1-capacity loss per cycle)$^{N-1}$

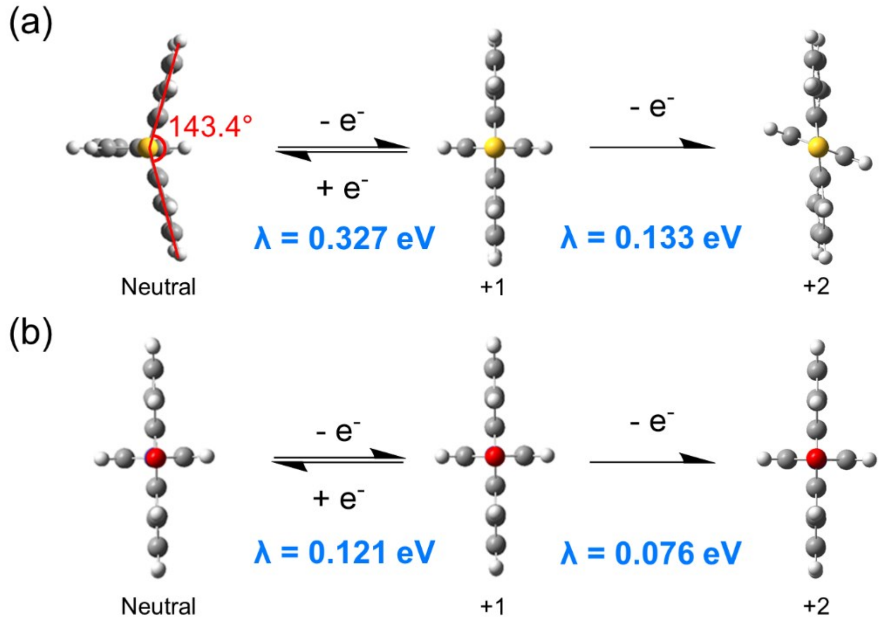


Fig. S39 Optimized molecular structures of the neutral, +1, and +2 charged states for (a) PhPTZ and (b) PhPXZ with reorganization energies (λ) for their redox reactions.

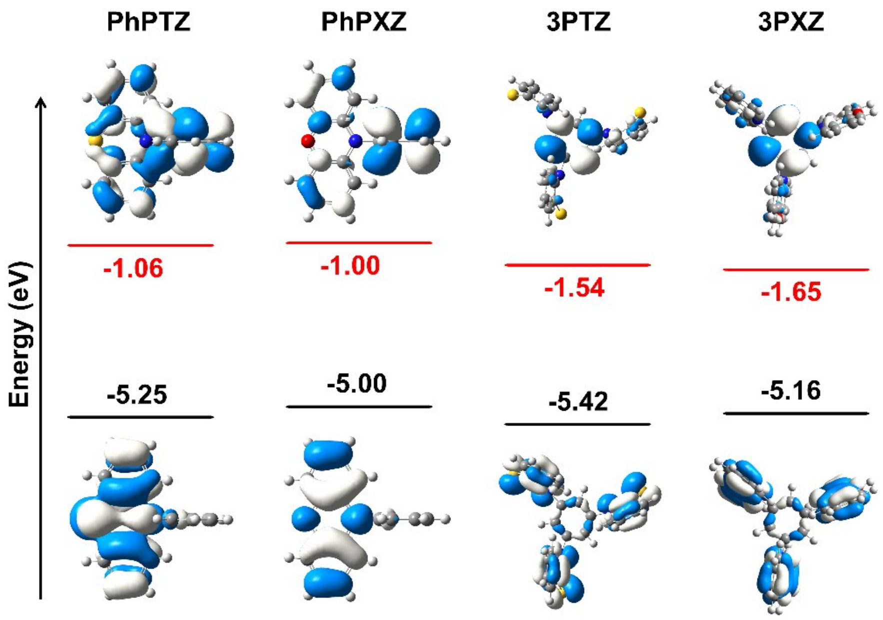


Fig. S40 DFT calculated HOMO (black) and LUMO (red) energy levels of PhPTZ, PhPXZ, 3PTZ, and 3PXZ, and corresponding molecular orbital plots.

2.10 The optimized geometries (x, y, z) of 3PTZ, 3PXZ, PhPTZ, and PhPXZ

3PTZ Neutral

C	0.47770	1.31041	-0.00002
C	-0.89793	1.06963	-0.00001
C	-1.37306	-0.24143	0.00001
C	-0.47672	-1.31236	0.00001
C	0.89621	-1.06834	-0.00002
C	1.37551	0.24341	-0.00003
N	2.78180	0.53444	-0.00006
N	-1.85318	2.14191	-0.00001
N	-0.92799	-2.67571	0.00004
C	3.48255	0.51010	1.23558
C	4.71940	1.16843	1.35277
S	5.32790	2.15344	-0.00013
C	4.71941	1.16830	-1.35293
C	3.48255	0.50999	-1.23569
C	-2.18289	2.76078	-1.23561
C	-3.37222	3.50151	-1.35281
S	-4.52965	3.53416	0.00002
C	-3.37216	3.50158	1.35279
C	-2.18283	2.76085	1.23558
C	-1.29948	-3.27048	-1.23554
C	-1.34741	-4.67081	-1.35273
S	-0.79786	-5.69002	0.00007
C	-1.34727	-4.67078	1.35289
C	-1.29936	-3.27045	1.23567
C	-1.36039	2.64796	-2.36423
C	-1.71400	3.25210	-3.56941
C	-2.87878	4.00590	-3.66716
C	-3.69875	4.13749	-2.54862
C	-3.69863	4.13762	2.54859
C	-2.87862	4.00609	3.66710
C	-1.71385	3.25228	3.56934
C	-1.36029	2.64807	2.36417
C	-1.61245	-2.50161	-2.36423
C	-1.95921	-3.10970	-3.56942
C	-2.03064	-4.49527	-3.66716
C	-1.73528	-5.27132	-2.54855
C	-1.73502	-5.27126	2.54877
C	-2.03027	-4.49518	3.66738
C	-1.95887	-3.10961	3.56960
C	-1.61224	-2.50155	2.36436
C	2.97284	-0.14491	2.36438
C	3.67261	-0.14097	3.56970
C	4.90841	0.48966	3.66746
C	5.43319	1.13293	2.54872
C	5.43320	1.13269	-2.54887
C	4.90842	0.48932	-3.66756
C	3.67261	-0.14128	-3.56975
C	2.97283	-0.14512	-2.36443
H	0.85801	2.32480	-0.00004
H	-2.44169	-0.41929	0.00003
H	1.58456	-1.90487	-0.00002
H	-0.44149	2.08102	-2.30840
H	-1.06169	3.13891	-4.42759
H	-3.14969	4.48812	-4.59867
H	-4.61134	4.72012	-2.60275
H	-4.61122	4.72025	2.60272
H	-3.14950	4.48835	4.59859
H	-1.06151	3.13913	4.42749
H	-0.44139	2.08113	2.30833
H	-1.58034	-1.42237	-2.30845
H	-2.18684	-2.48802	-4.42760
H	-2.31310	-4.97082	-4.59866
H	-1.78440	-6.35293	-2.60260
H	-1.78412	-6.35287	2.60286
H	-2.31264	-4.97071	4.59893
H	-2.18644	-2.48791	4.42779
H	-1.58015	-1.42231	2.30854
H	2.02201	-0.65649	2.30857
H	3.24773	-0.64855	4.42796
H	5.46131	0.48298	4.59906
H	6.39459	1.63094	2.60278
H	6.39460	1.63068	-2.60297
H	5.46132	0.48256	-4.59916
H	3.24773	-0.64892	-4.42798
H	2.02200	-0.65667	-2.30859

3PTZ (+1)

C	0.0057	1.3969	0.0000
C	-1.2066	0.7038	0.0000
C	-1.2119	-0.6900	0.0001
C	-0.0056	-1.3934	0.0001
C	1.2042	-0.7010	0.0001
C	1.2102	0.6953	0.0001
N	2.4382	1.4441	0.0000
N	-2.4693	1.3918	0.0000
N	0.0298	-2.8311	0.0001
C	3.1091	1.6471	1.2353
C	4.0744	2.6632	1.3542
S	4.3428	3.7898	-0.0002
C	4.0744	2.6629	-1.3544
C	3.1091	1.6468	-1.2353
C	-2.9820	1.8692	-1.2353
C	-4.3461	2.1911	-1.3548
S	-5.4543	1.8552	-0.0001
C	-4.3461	2.1911	1.3547
C	-2.9821	1.8692	1.2352
C	-0.1287	-3.5140	-1.2353
C	0.2730	-4.8567	-1.3544
S	1.1175	-5.6491	0.0000
C	0.2730	-4.8567	1.3545
C	-0.1286	-3.5140	1.2354
C	-2.1679	2.0203	-2.3665
C	-2.6970	2.4764	-3.5729
C	-4.0423	2.8194	-3.6718
C	-4.8612	2.6849	-2.5521
C	-4.8613	2.6850	2.5520
C	-4.0424	2.8195	3.6717
C	-2.6971	2.4765	3.5729
C	-2.1680	2.0204	2.3665
C	-0.6651	-2.8842	-2.3670
C	-0.7965	-3.5707	-3.5732
C	-0.4229	-4.9079	-3.6714
C	0.1020	-5.5500	-2.5514
C	0.1021	-5.5500	2.5516
C	-0.4228	-4.9079	3.6716
C	-0.7964	-3.5707	3.5733
C	-0.6650	-2.8842	2.3672
C	2.8297	0.8688	2.3674
C	3.4906	1.0966	3.5736
C	4.4652	2.0854	3.6714
C	4.7612	2.8596	2.5510
C	4.7612	2.8590	-2.5513
C	4.4652	2.0845	-3.6715
C	3.4906	1.0957	-3.5734
C	2.8297	0.8682	-2.3672
H	0.0195	2.4798	0.0000
H	-2.1569	-1.2193	0.0000
H	2.1349	-1.2547	0.0000
H	-1.1169	1.7740	-2.3124
H	-2.0433	2.5724	-4.4321
H	-4.4539	3.1858	-4.6045
H	-5.9128	2.9421	-2.6089
H	-5.9129	2.9422	2.6087
H	-4.4541	3.1859	4.6044
H	-2.0435	2.5726	4.4321
H	-1.1170	1.7740	2.3125
H	-0.9753	-1.8501	-2.3138
H	-1.2053	-3.0523	-4.4327
H	-0.5349	-5.4477	-4.6039
H	0.4037	-6.5897	-2.6076
H	0.4038	-6.5897	2.6078
H	-0.5347	-5.4477	4.6041
H	-1.2051	-3.0523	4.4329
H	-0.9752	-1.8501	2.3140
H	2.0876	0.0847	2.3142
H	3.2445	0.4840	4.4331
H	4.9896	2.2567	4.6037
H	5.5135	3.6382	2.6068
H	5.5135	3.6376	-2.6072
H	4.9896	2.2556	-4.6039
H	3.2445	0.4830	-4.4328
H	2.0876	0.0841	-2.3138

3PTZ (+2)

C	0.01746	1.42557	-0.00015
C	-1.19644	0.74005	-0.00008
C	-1.22333	-0.65512	-0.00002
C	-0.02183	-1.36533	0.00000
C	1.19908	-0.68997	-0.00006
C	1.21143	0.70525	-0.00014
N	2.46647	1.42235	-0.00016
N	-2.45183	1.45751	-0.00005
N	-0.01925	-2.80561	0.00011
C	3.04420	1.72891	1.24710
C	4.16032	2.59225	1.36415
S	4.91007	3.39014	-0.00021
C	4.16043	2.59203	-1.36451
C	3.04431	1.72870	-1.24741
C	-3.02745	1.77077	-1.24689
C	-4.37000	2.20304	-1.36433
S	-5.45663	2.35004	0.00009
C	-4.36982	2.20322	1.36438
C	-3.02727	1.77095	1.24681
C	-0.03182	-3.46428	-1.24769
C	0.25072	-4.84491	-1.36388
S	0.69178	-5.85413	0.00025
C	0.25090	-4.84475	1.36431
C	-0.03158	-3.46411	1.24799
C	-2.27247	1.65393	-2.42942
C	-2.82465	1.95057	-3.66456
C	-4.15338	2.37580	-3.76884
C	-4.91474	2.50157	-2.62149
C	-4.91440	2.50188	2.62157
C	-4.15289	2.37625	3.76884
C	-2.82417	1.95100	3.66444
C	-2.27215	1.65423	2.42926
C	-0.31905	-2.75228	-2.42707
C	-0.32439	-3.38227	-3.66145
C	-0.04420	-4.74797	-3.76488
C	0.23803	-5.46938	-2.61837
C	0.23838	-5.46905	2.61888
C	-0.04357	-4.74747	3.76536
C	-0.32362	-3.38176	3.66181
C	-0.31849	-2.75193	2.42735
C	2.51243	1.18533	2.43239
C	3.06092	1.48554	3.66814
C	4.16272	2.34143	3.77174
C	4.70503	2.88603	2.62257
C	4.70527	2.88560	-2.62293
C	4.16308	2.34079	-3.77206
C	3.06129	1.48489	-3.66842
C	2.51269	1.18489	-2.43267
H	0.03420	2.50908	-0.00020
H	-2.16975	-1.18270	0.00007
H	2.12865	-1.24667	-0.00002
H	-1.23955	1.34332	-2.37773
H	-2.21411	1.86065	-4.55470
H	-4.58296	2.61173	-4.73406
H	-5.94408	2.83597	-2.68357
H	-5.94374	2.83627	2.68375
H	-4.58234	2.61227	4.73409
H	-2.21352	1.86117	4.55451
H	-1.23924	1.34357	2.37747
H	-0.55549	-1.69974	-2.37540
H	-0.55917	-2.80870	-4.54975
H	-0.05367	-5.24188	-4.72813
H	0.45081	-6.53052	-2.68036
H	0.45108	-6.53021	2.68097
H	-0.05291	-5.24126	4.72867
H	-0.55814	-2.80804	4.55009
H	-0.55481	-1.69937	2.37559
H	1.67197	0.50945	2.38317
H	2.63415	1.04285	4.55979
H	4.59325	2.57235	4.73773
H	5.56276	3.54620	2.68382
H	5.56299	3.54577	-2.68421
H	4.59370	2.57155	-4.73804
H	2.63463	1.04201	-4.56003
H	1.67224	0.50898	-2.38341

3PTZ (+3)

C	1.32261	-0.46085	-0.00028
C	1.05276	0.90862	-0.00006
C	-0.2622	1.37655	0.00012
C	-1.31318	0.45808	0.0001
C	-1.06097	-0.91467	-0.00013
C	0.25993	-1.36572	-0.00031
N	0.53091	-2.79341	-0.00045
N	2.15376	1.85704	0.00002
N	-2.68509	0.93726	0.00032
C	0.65166	-3.43191	1.24527
C	0.90775	-4.82547	1.35851
S	1.09856	-5.88775	-0.0007
C	0.90717	-4.82535	-1.35974
C	0.6512	-3.43178	-1.24628
C	2.64649	2.28063	-1.24571
C	3.72573	3.19867	-1.35902
S	4.55032	3.89513	0.00014
C	3.72615	3.19802	1.35922
C	2.64686	2.28002	1.24579
C	-3.2984	1.15232	-1.2453
C	-4.63321	1.62759	-1.35851
S	-5.64856	1.99339	0.00076
C	-4.63311	1.62674	1.35973
C	-3.29827	1.15164	1.24613
C	2.07672	1.80037	-2.44256
C	2.55178	2.20802	-3.67508
C	3.61852	3.11465	-3.77426
C	4.1965	3.60255	-2.62208
C	4.19734	3.60124	2.62233
C	3.61979	3.11273	3.77445
C	2.55305	2.2061	3.67516
C	2.07756	1.79908	2.4426
C	-2.59752	0.89949	-2.4422
C	-3.18824	1.10683	-3.67468
C	-4.50697	1.57681	-3.77377
C	-5.21851	1.83317	-2.62154
C	-5.21833	1.83149	2.62293
C	-4.50668	1.5745	3.77495
C	-3.1879	1.10473	3.67548
C	-2.59726	0.89817	2.44282
C	0.52011	-2.69854	2.4422
C	0.63624	-3.31377	3.67466
C	0.88899	-4.69073	3.77375
C	1.02272	-5.43509	2.62151
C	1.02157	-5.43488	-2.62285
C	0.88739	-4.69043	-3.77496
C	0.63476	-3.31346	-3.67566
C	0.51918	-2.69832	-2.4431
H	2.34608	-0.81751	-0.00038
H	-0.46506	2.44125	0.00029
H	-1.88185	-1.6224	-0.00013
H	1.25439	1.1028	-2.40367
H	2.09229	1.82128	-4.5765
H	3.98532	3.42954	-4.74297
H	5.02137	4.30417	-2.67848
H	5.02223	4.30284	2.67881
H	3.98692	3.4271	4.7432
H	2.09391	1.81883	4.57654
H	1.25529	1.10146	2.40363
H	-1.58202	0.53674	-2.40333
H	-2.62349	0.90266	-4.57615
H	-4.96321	1.73686	-4.74245
H	-6.23868	2.1964	-2.67787
H	-6.23853	2.19458	2.67956
H	-4.96285	1.73389	4.74376
H	-2.62305	0.90008	4.57677
H	-1.58174	0.53552	2.40365
H	0.32596	-1.63781	2.4035
H	0.53059	-2.72258	4.5761
H	0.97876	-5.16583	4.74242
H	1.21844	-6.50016	2.67782
H	1.21719	-6.49996	-2.67932
H	0.97669	-5.16545	-4.74371
H	0.52877	-2.72219	-4.57701
H	0.32507	-1.63759	-2.40423

3PXZ Neutral

C	0.85781	1.10165	-0.00953
C	-0.52466	1.29318	-0.00480
C	-1.38105	0.19114	0.00292
C	-0.85552	-1.10186	0.00594
C	0.52705	-1.29263	0.00202
C	1.38400	-0.19102	-0.00553
N	2.80120	-0.38628	-0.00865
N	-1.06317	2.61850	-0.00665
N	-1.73378	-2.23111	0.01332
C	3.52350	-0.34285	-1.21943
C	4.91524	-0.53252	-1.19152
O	5.59737	-0.76135	-0.01358
C	4.88161	-0.81426	1.16545
C	3.48929	-0.62958	1.19844
C	-1.17781	3.34206	1.19885
C	-1.70788	4.64272	1.16695
O	-2.12191	5.23370	-0.00967
C	-2.01217	4.51675	-1.18403
C	-1.48770	3.21372	-1.21304
C	-2.05476	-2.89171	-1.19097
C	-2.92241	-3.99606	-1.15378
O	-3.47276	-4.45272	0.02679
C	-3.15345	-3.80094	1.20084
C	-2.28984	-2.69309	1.22455
C	-0.79246	2.82131	2.43685
C	-0.92501	3.57439	3.60510
C	-1.44800	4.85994	3.55474
C	-1.84102	5.39083	2.32495
C	-2.44025	5.14279	-2.34297
C	-2.35571	4.48422	-3.57091
C	-1.83647	3.19704	-3.61844
C	-1.40484	2.56771	-2.44919
C	-1.55233	-2.49417	-2.43267
C	-1.89837	-3.17840	-3.59956
C	-2.75485	-4.27021	-3.54399
C	-3.26726	-4.67557	-2.31036
C	-3.72216	-4.29112	2.36473
C	-3.44339	-3.68785	3.59237
C	-2.58908	-2.59374	3.63461
C	-2.01604	-2.10146	2.46038
C	2.91616	-0.12427	-2.45862
C	3.67186	-0.08952	-3.63219
C	5.04730	-0.27591	-3.58588
C	5.66629	-0.49954	-2.35477
C	5.60025	-1.05413	2.32491
C	4.94752	-1.11528	3.55737
C	3.57192	-0.93151	3.60879
C	2.84910	-0.68955	2.43894
H	1.52292	1.95679	-0.01541
H	-2.45422	0.33941	0.00687
H	0.93514	-2.29620	0.00502
H	-0.38302	1.82153	2.48877
H	-0.61506	3.14431	4.55003
H	-1.55372	5.45065	4.45632
H	-2.25548	6.38850	2.24411
H	-2.83677	6.14790	-2.26441
H	-2.69300	4.97913	-4.47327
H	-1.76171	2.66959	-4.56192
H	-1.00276	1.56485	-2.49895
H	-0.88365	-1.64585	-2.48861
H	-1.49079	-2.84794	-4.54751
H	-3.02778	-4.80651	-4.44446
H	-3.93980	-5.52064	-2.22544
H	-4.38141	-5.14755	2.29019
H	-3.89220	-4.07548	4.49861
H	-2.35967	-2.11231	4.57776
H	-1.35271	-1.24833	2.50587
H	1.84568	0.02290	-2.50723
H	3.17291	0.08460	-4.57806
H	5.64058	-0.25008	-4.49159
H	6.73613	-0.65140	-2.27698
H	6.67197	-1.18977	2.24321
H	5.51530	-1.30382	4.46017
H	3.04724	-0.97449	4.55579
H	1.77797	-0.54878	2.49165

3PXZ (+1)

C	-0.5656	1.2857	-0.0247
C	-1.3829	0.1592	-0.0241
C	-0.8264	-1.1249	-0.0273
C	0.5520	-1.2663	-0.0316
C	1.3827	-0.1485	-0.0509
C	0.8211	1.1189	-0.0379
N	1.6659	2.2716	-0.0206
N	-2.8075	0.3113	-0.0088
N	1.1304	-2.5812	-0.0169
C	1.8222	3.0540	-1.1826
C	2.5767	4.2349	-1.1077
O	3.1421	4.6636	0.0766
C	3.1626	3.7632	1.1420
C	2.3403	2.6249	1.1587
C	-3.4915	0.4264	1.2166
C	-4.8932	0.5160	1.1921
O	-5.6047	0.5029	0.0211
C	-4.9284	0.4128	-1.1746
C	-3.5173	0.3124	-1.2100
C	1.4800	-3.2148	-1.2233
C	2.0812	-4.4824	-1.1695
O	2.3303	-5.1107	0.0216
C	1.9936	-4.4793	1.1977
C	1.3924	-3.2119	1.2036
C	-2.8383	0.4573	2.4509
C	-3.5636	0.5545	3.6274
C	-4.9619	0.6325	3.5947
C	-5.6255	0.6129	2.3751
C	-5.6769	0.4267	-2.3327
C	-5.0494	0.3416	-3.5769
C	-3.6612	0.2435	-3.6304
C	-2.9004	0.2295	-2.4693
C	1.2482	-2.6384	-2.4777
C	1.6073	-3.3085	-3.6349
C	2.2025	-4.5642	-3.5726
C	2.4387	-5.1597	-2.3334
C	2.2731	-5.1545	2.3849
C	1.9474	-4.5675	3.5998
C	1.3507	-3.3032	3.6333
C	1.0700	-2.6350	2.4429
C	1.2544	2.6975	-2.4136
C	1.4525	3.4988	-3.5294
C	2.2094	4.6589	-3.4484
C	2.7724	5.0344	-2.2303
C	3.8555	4.1690	2.2655
C	3.7390	3.4294	3.4567
C	2.9261	2.2946	3.4928
C	2.2321	1.8928	2.3578
H	-1.0000	2.2734	-0.0117
H	-1.4686	-1.9943	-0.0167
H	2.4605	-0.2747	-0.0549
H	-1.7524	0.3998	2.4858
H	-3.0461	0.5776	4.5786
H	-5.5247	0.7157	4.5099
H	-6.7020	0.6806	2.3061
H	-6.7620	0.5078	-2.2550
H	-5.6345	0.3577	-4.4779
H	-3.1566	0.1702	-4.5859
H	-1.8247	0.1508	-2.5231
H	0.7951	-1.6576	-2.5420
H	1.4315	-2.8394	-4.5962
H	2.4868	-5.0882	-4.4781
H	2.9017	-6.1312	-2.2447
H	2.7386	-6.1338	2.3270
H	2.1657	-5.0913	4.5300
H	1.0887	-2.8443	4.5787
H	0.6033	-1.6559	2.4775
H	0.6606	1.7928	-2.4829
H	1.0003	3.2062	-4.4722
H	2.3682	5.2825	-4.3228
H	3.3732	5.9342	-2.1288
H	4.2972	5.1586	2.2352
H	4.1261	3.8544	4.3752
H	2.8551	1.7000	4.4087
H	1.6934	0.9405	2.3680

3PXZ (+2)

C	1.21245	-0.66543	0.01746
C	0.00034	-1.35759	-0.00007
C	-1.21214	-0.66606	-0.01758
C	-1.20367	0.72980	-0.01519
C	-0.00039	1.43422	-0.00003
C	1.20325	0.73043	0.01511
N	2.45416	1.44428	0.02140
N	0.00071	-2.79158	-0.00008
N	-2.45495	1.44300	-0.02140
C	3.15908	1.60838	1.22105
C	4.41110	2.26337	1.18791
O	4.93444	2.73488	0.02240
C	4.24746	2.57908	-1.14349
C	2.99399	1.92813	-1.17884
C	0.20078	-3.49567	-1.19854
C	0.19818	-4.90678	-1.16319
O	0.00147	-5.59073	-0.00007
C	-0.19560	-4.90688	1.16306
C	-0.19896	-3.49577	1.19839
C	-2.99497	1.92650	1.17888
C	-4.24877	2.57684	1.14363
O	-4.93585	2.73240	-0.02222
C	-4.41231	2.26125	-1.18779
C	-3.15998	1.60686	-1.22102
C	0.39562	-2.86256	-2.43518
C	0.58874	-3.61547	-3.58405
C	0.58889	-5.01457	-3.52834
C	0.39150	-5.65905	-2.31624
C	-0.38850	-5.65925	2.31612
C	-0.58622	-5.01486	3.52822
C	-0.58684	-3.61576	3.58391
C	-0.39414	-2.86275	2.43503
C	-2.35210	1.79241	2.41906
C	-2.94001	2.29710	3.56851
C	-4.18199	2.94447	3.51246
C	-4.83631	3.08234	2.29853
C	-5.15887	2.45669	-2.34456
C	-4.66627	2.00321	-3.55831
C	-3.42352	1.35724	-3.61267
C	-2.67669	1.16144	-2.46151
C	2.67597	1.16261	2.46148
C	3.42267	1.35866	3.61268
C	4.66512	2.00523	3.55841
C	5.15754	2.45905	2.34472
C	4.83480	3.08497	-2.29832
C	4.18060	2.94688	-3.51229
C	2.93894	2.29891	-3.56844
C	2.35123	1.79383	-2.41905
H	2.15040	-1.20756	0.03055
H	-2.14980	-1.20869	-0.03067
H	-0.00067	2.51777	0.00001
H	0.39687	-1.78305	-2.49317
H	0.73980	-3.11339	-4.53146
H	0.74041	-5.59613	-4.42875
H	0.38182	-6.73891	-2.23686
H	-0.37823	-6.73910	2.23675
H	-0.73740	-5.59650	4.42864
H	-0.73815	-3.11375	4.53132
H	-0.39597	-1.78324	2.49301
H	-1.39388	1.29575	2.47774
H	-2.43186	2.18886	4.51855
H	-4.63328	3.33614	4.41515
H	-5.79814	3.57311	2.21796
H	-6.11295	2.96268	-2.26603
H	-5.24276	2.15159	-4.46251
H	-3.03983	1.00739	-4.56285
H	-1.71944	0.66270	-2.51837
H	1.71895	0.66342	2.51826
H	3.03911	1.00855	4.56282
H	5.24151	2.15379	4.46264
H	6.11137	2.96550	2.26626
H	5.79639	3.57620	-2.21768
H	4.63172	3.33885	-4.41493
H	2.43087	2.19049	-4.51850
H	1.39326	1.29670	-2.47781

3PXZ (+3)

C	-0.28274	-1.37348	0.00169
C	-1.31887	-0.43826	0.00074
C	-1.04828	0.93106	-0.00069
C	0.27965	1.36072	-0.00164
C	1.33016	0.44169	-0.00101
C	1.03838	-0.92323	0.00086
N	2.12128	-1.88535	0.00176
N	-2.69356	-0.89486	0.00151
N	0.57161	2.77952	-0.00338
C	2.56697	-2.43113	1.20853
C	3.62862	-3.37180	1.17415
O	4.20386	-3.73412	0.00350
C	3.77698	-3.20689	-1.16799
C	2.71712	-2.26432	-1.20414
C	-3.31796	-1.22651	-1.20387
C	-4.66447	-1.67230	-1.16778
O	-5.33647	-1.77247	0.00312
C	-4.73676	-1.45039	1.17325
C	-3.39102	-1.00216	1.20770
C	0.82482	3.43982	1.20195
C	1.11009	4.82918	1.16503
O	1.13392	5.50697	-0.00657
C	0.88707	4.87241	-1.17661
C	0.59929	3.48345	-1.21025
C	-2.68216	-1.13816	-2.45483
C	-3.36782	-1.48587	-3.60412
C	-4.70323	-1.92935	-3.54613
C	-5.35151	-2.02160	-2.32913
C	-5.49511	-1.58073	2.33545
C	-4.91920	-1.26611	3.55167
C	-3.58370	-0.82269	3.60804
C	-2.82735	-0.69203	2.45791
C	0.80834	2.79940	2.45360
C	1.07067	3.52228	3.60274
C	1.35503	4.90033	3.54391
C	1.37379	5.55363	2.32624
C	0.93069	5.63944	-2.33958
C	0.68852	5.02931	-3.55571
C	0.40416	3.65111	-3.61125
C	0.35997	2.88600	-2.46036
C	2.02012	-2.09403	2.45924
C	2.51578	-2.67888	3.60998
C	3.56830	-3.61289	3.55370
C	4.12502	-3.95850	2.33695
C	4.41969	-3.63093	-2.32983
C	4.01182	-3.11989	-3.54735
C	2.95957	-2.18567	-3.60537
C	2.31882	-1.76215	-2.45559
H	-0.50123	-2.43511	0.00295
H	-1.85845	1.65106	-0.00093
H	2.35875	0.78341	-0.00215
H	-1.65769	-0.80000	-2.51844
H	-2.87134	-1.41628	-4.56403
H	-5.22447	-2.19775	-4.45655
H	-6.37824	-2.35641	-2.24649
H	-6.51828	-1.92657	2.25404
H	-5.49655	-1.36222	4.46273
H	-3.14327	-0.58084	4.56735
H	-1.80398	-0.35034	2.52024
H	0.59180	1.74257	2.51779
H	1.05724	3.02217	4.56319
H	1.55839	5.45041	4.45421
H	1.58642	6.61239	2.24299
H	1.15434	6.69612	-2.25888
H	0.71872	5.61292	-4.46734
H	0.21771	3.18439	-4.57050
H	0.14023	1.82967	-2.52200
H	1.21199	-1.37921	2.52141
H	2.08900	-2.41523	4.56972
H	3.94363	-4.06103	4.46523
H	4.93647	-4.67127	2.25564
H	5.22364	-4.35200	-2.24718
H	4.50233	-3.43996	-4.45814
H	2.64818	-1.79378	-4.56569
H	1.51331	-1.04447	-2.51912

PhPTZ Neutral

C	-2.32555	0.00023	1.39603
C	-4.47708	0.00040	0.29731
C	-2.44934	0.00022	-1.01639
C	-1.68840	0.00018	0.15570
N	-0.24889	0.00006	0.11748
C	0.41806	1.23634	-0.08645
C	1.79559	1.35305	0.17474
C	1.79527	-1.35341	0.17474
C	0.41778	-1.23638	-0.08644
C	-0.26397	2.37788	-0.53111
C	0.40445	3.58647	-0.71618
C	1.77335	3.68053	-0.48978
C	2.46543	2.55316	-0.05318
C	2.46482	-2.55369	-0.05319
C	1.77246	-3.68088	-0.48980
C	0.40358	-3.58649	-0.71619
C	-0.26455	-2.37774	-0.53111
H	-1.72204	0.00019	2.29603
H	-5.55976	0.00048	0.35214
H	-1.94854	0.00017	-1.97786
H	-1.32682	2.32824	-0.72070
H	-0.15580	4.45263	-1.04927
H	2.29893	4.61500	-0.64538
H	3.53179	2.60335	0.13602
H	3.53116	-2.60414	0.13601
H	2.29781	-4.61549	-0.64540
H	-0.15689	-4.45251	-1.04929
H	-1.32738	-2.32782	-0.72071
C	-3.71796	0.00034	1.46607
H	-4.20763	0.00039	2.43324
C	-3.84089	0.00033	-0.94384
H	-4.42725	0.00037	-1.85576
S	2.67603	-0.00029	0.92394

PhPTZ (+1)

C	-2.3663	-0.0011	1.2153
C	-4.4549	-0.0020	-0.0006
C	-2.3658	-0.0011	-1.2154
C	-1.6866	-0.0009	0.0001
N	-0.2272	-0.0002	0.0004
C	0.4153	1.2392	0.0003
C	1.8302	1.3632	-0.0001
C	1.8318	-1.3614	-0.0001
C	0.4167	-1.2390	0.0003
C	-0.3475	2.4300	0.0005
C	0.2660	3.6651	0.0004
C	1.6660	3.7742	0.0000
C	2.4366	2.6301	-0.0002
C	2.4396	-2.6275	-0.0002
C	1.6704	-3.7726	0.0000
C	0.2702	-3.6652	0.0004
C	-0.3446	-2.4307	0.0005
H	-1.8159	-0.0009	2.1489
H	-5.5382	-0.0024	-0.0008
H	-1.8149	-0.0009	-2.1488
H	-1.4250	2.3708	0.0008
H	-0.3458	4.5588	0.0006
H	2.1403	4.7475	-0.0002
H	3.5185	2.6976	-0.0006
H	3.5216	-2.6938	-0.0006
H	2.1458	-4.7453	-0.0002
H	-0.3405	-4.5596	0.0006
H	-1.4223	-2.3728	0.0008
C	-3.7602	-0.0017	1.2086
H	-4.3000	-0.0019	2.1477
C	-3.7596	-0.0017	-1.2093
H	-4.2989	-0.0019	-2.1488
S	2.9139	0.0015	-0.0003

PhPTZ (+2)

C	2.38295	0.51451	-1.11336
C	4.46541	-0.00215	-0.00117
C	2.38332	-0.51699	1.11260
C	1.69778	-0.00098	-0.00016
N	0.25097	-0.00034	0.00020
C	-0.40990	1.23686	0.05066
C	-1.82283	1.35451	-0.03581
C	-1.82466	-1.35234	0.03506
C	-0.41144	-1.23672	-0.04983
C	0.32563	2.42259	0.22868
C	-0.29765	3.67760	0.19816
C	-1.67454	3.78353	0.04446
C	-2.43849	2.61911	-0.04741
C	-2.44213	-2.61607	0.04703
C	-1.67971	-3.78165	-0.04269
C	-0.30250	-3.67778	-0.19483
C	0.32258	-2.42367	-0.22593
H	1.83444	0.88266	-1.97258
H	5.54908	-0.00270	-0.00158
H	1.83507	-0.88461	1.97221
H	1.38869	2.37273	0.41602
H	0.30978	4.56700	0.31565
H	-2.16003	4.75135	0.02555
H	-3.51947	2.68502	-0.11497
H	-3.52329	-2.68038	0.11321
H	-2.16658	-4.74877	-0.02340
H	0.30386	-4.56813	-0.31067
H	1.38590	-2.37556	-0.41222
C	3.76993	0.49480	-1.11253
H	4.31405	0.85704	-1.97627
C	3.77029	-0.49855	1.11071
H	4.31474	-0.86138	1.97399
S	-2.90670	0.00178	-0.00176

PhPXZ Neutral

C	-4.38234	-0.00005	-0.03299
C	-2.25170	-0.00015	-1.17131
C	-1.59478	-0.00003	0.06080
C	-2.33233	0.00008	1.24489
N	-0.16164	-0.00001	0.11642
C	0.54874	1.21429	0.03751
C	1.95336	1.18551	0.06335
O	2.65196	0.00004	0.18604
C	1.95340	-1.18546	0.06336
C	0.54878	-1.21428	0.03752
C	-0.08111	2.45867	-0.05383
C	0.66689	3.63625	-0.11543
C	2.05508	3.58924	-0.09365
C	2.69657	2.35190	-0.00629
C	2.69664	-2.35182	-0.00626
C	2.05520	-3.58918	-0.09360
C	0.66701	-3.63624	-0.11535
C	-0.08103	-2.45869	-0.05377
H	-5.46580	-0.00006	-0.06958
H	-1.66743	-0.00023	-2.08429
H	-1.80811	0.00017	2.19343
H	-1.16183	2.50575	-0.07146
H	0.15127	4.58708	-0.18139
H	2.64109	4.49888	-0.14252
H	3.77689	2.27301	0.01621
H	3.77696	-2.27290	0.01623
H	2.64124	-4.49880	-0.14246
H	0.15142	-4.58709	-0.18128
H	-1.16175	-2.50580	-0.07138
C	-3.64436	-0.00016	-1.21645
H	-4.15227	-0.00026	-2.17421
C	-3.72565	0.00007	1.19666
H	-4.29626	0.00016	2.11839

PhPXZ (+1)

C	-4.36723	0.00000	0.00052
C	-2.27965	-0.00012	-1.21666
C	-1.60162	0.00000	-0.00011
C	-2.27910	0.00012	1.21679
N	-0.14703	0.00000	-0.00037
C	0.54547	1.20363	-0.00026
C	1.96166	1.17663	0.00013
O	2.64103	0.00000	0.00023
C	1.96166	-1.17663	0.00014
C	0.54547	-1.20363	-0.00024
C	-0.10277	2.45436	-0.00060
C	0.64522	3.61467	-0.00045
C	2.05153	3.56724	0.00007
C	2.71013	2.34997	0.00035
C	2.71012	-2.34997	0.00036
C	2.05152	-3.56725	0.00012
C	0.64522	-3.61467	-0.00037
C	-0.10278	-2.45436	-0.00053
H	-5.45058	0.00000	0.00083
H	-1.72921	-0.00021	-2.15020
H	-1.72827	0.00021	2.15010
H	-1.18279	2.49476	-0.00091
H	0.14023	4.57244	-0.00074
H	2.62318	4.48681	0.00026
H	3.79041	2.27955	0.00073
H	3.79041	-2.27956	0.00074
H	2.62317	-4.48681	0.00032
H	0.14023	-4.57244	-0.00063
H	-1.18279	-2.49476	-0.00081
C	-3.67330	-0.00012	-1.20892
H	-4.21346	-0.00020	-2.14785
C	-3.67273	0.00012	1.20967
H	-4.21248	0.00021	2.14882

PhPXZ (+2)

C	4.38380	0.00000	0.00016
C	2.29705	0.00003	-1.22296
C	1.62659	0.00000	0.00005
C	2.29696	-0.00003	1.22310
N	0.16316	0.00000	-0.00001
C	-0.54253	-1.19522	-0.00005
C	-1.95811	-1.16849	-0.00006
O	-2.63492	0.00000	-0.00003
C	-1.95811	1.16849	-0.00002
C	-0.54253	1.19522	-0.00001
C	0.08942	-2.45116	-0.00008
C	-0.67818	-3.63448	-0.00013
C	-2.06715	-3.58557	-0.00014
C	-2.71992	-2.34456	-0.00010
C	-2.71992	2.34456	-0.00001
C	-2.06715	3.58557	0.00000
C	-0.67818	3.63448	0.00001
C	0.08942	2.45116	0.00001
H	5.46710	0.00000	0.00020
H	1.75102	0.00005	-2.15962
H	1.75085	-0.00005	2.15972
H	1.17066	-2.50430	-0.00007
H	-0.16566	-4.58910	-0.00016
H	-2.65113	-4.49778	-0.00017
H	-3.80160	-2.26733	-0.00011
H	-3.80160	2.26733	-0.00002
H	-2.65113	4.49778	0.00000
H	-0.16566	4.58910	0.00002
H	1.17066	2.50430	0.00002
C	3.69102	0.00003	-1.21079
H	4.23177	0.00005	-2.14949
C	3.69092	-0.00003	1.21105
H	4.23160	-0.00005	2.14979

3 References

1 N. J. Treat, H. Sprafke, J. W. Kramer, P. G. Clark, B. E. Barton, J. Read De Alaniz, B. P. Fors and C. J. Hawker, Metal-free atom transfer radical polymerization, *J. Am. Chem. Soc.*, 2014, **136**, 16096–16101.

2 N. Liu, B. Wang, W. Chen, C. Liu, X. Wang and Y. Hu, A general route for synthesis of N-aryl phenoxazines via copper(i)-catalyzed N-, N-, and O-arylations of 2-aminophenols, *RSC Adv.*, 2014, **4**, 51133–51139.

3 W. Kam, C.-W. Liew, J. Y. Lim and S. Ramesh, Electrical, structural, and thermal studies of antimony trioxide-doped poly(acrylic acid)-based composite polymer electrolytes, *Ionics (Kiel).*, 2014, **20**, 665–674.

4 M. Lee, J. Hong, B. Lee, K. Ku, S. Lee, C. B. Park and K. Kang, Multi-electron redox phenazine for ready-to-charge organic batteries, *Green Chem.*, 2017, **19**, 2980–2985.

5 É. Deunf, P. Moreau, É. Quarez, D. Guyomard, F. Dolhem and P. Poizot, Reversible anion intercalation in a layered aromatic amine: a high-voltage host structure for organic batteries, *J. Mater. Chem. A*, 2016, **4**, 6131–6139.

6 S. Chen, T. Jia, G. Zhou, C. Zhang, Q. Hou, Y. Wang, S. Luo, G. Shi and Y. Zeng, A Cross-Linked Triphenylamine-Based Polymer Cathode Material with Dual Anion-Cation Reversible Insertion for Lithium Ion Battery, *J. Electrochem. Soc.*, 2019, **166**, A2543–A2548.

7 J. K. Kim, G. Cheruvally, J. H. Ahn, Y. G. Seo, D. S. Choi, S. H. Lee and C. E. Song, Organic radical battery with PTMA cathode: Effect of PTMA content on electrochemical properties, *J. Ind. Eng. Chem.*, 2008, **14**, 371–376.

8 M. E. Speer, M. Kolek, J. J. Jassoy, J. Heine, M. Winter, P. M. Bieker and B. Esser, Thianthrene-functionalized polynorbornenes as high-voltage materials for organic cathode-based dual-ion batteries, *Chem. Commun.*, 2015, **51**, 15261–15264.

9 B. M. Peterson, D. Ren, L. Shen, Y.-C. M. Wu, B. Ulgut, G. W. Coates, H. D. Abruña and B. P. Fors, Phenothiazine-Based Polymer Cathode Materials with Ultrahigh Power Densities for Lithium Ion Batteries, *ACS Appl. Energy Mater.*, 2018, **1**, 3560–3564.

10 F. A. Obrezkov, A. F. Shestakov, V. F. Traven, K. J. Stevenson and P. A. Troshin, An ultrafast charging polyphenylamine-based cathode material for high rate lithium, sodium and potassium batteries, *J. Mater. Chem. A*, 2019, **7**, 11430–11437.

11 G. Dai, X. Wang, Y. Qian, Z. Niu, X. Zhu, J. Ye, Y. Zhao and X. Zhang, Manipulation of conjugation to stabilize N redox-active centers for the design of high-voltage organic battery cathode, *Energy Storage Mater.*, 2019, **16**, 236–242.

12 F. Otteny, M. Kolek, J. Becking, M. Winter, P. Bieker and B. Esser, Unlocking Full Discharge Capacities of Poly(vinylphenothiazine) as Battery Cathode Material by Decreasing Polymer Mobility Through Cross-Linking, *Adv. Energy Mater.*, 2018, **8**, 1802151.

13 M. Kolek, F. Otteny, P. Schmidt, C. Mück-Lichtenfeld, C. Einholz, J. Becking, E.

Schleicher, M. Winter, P. Bieker and B. Esser, Ultra-high cycling stability of poly(vinylphenothiazine) as a battery cathode material resulting from π–π interactions, *Energy Environ. Sci.*, 2017, **10**, 2334–2341.

14 G. Dai, Y. Gao, Z. Niu, P. He, X. Zhang, Y. Zhao and H. Zhou, Dilution of the Electron Density in the π-Conjugated Skeleton of Organic Cathode Materials Improves the Discharge Voltage, *ChemSusChem*, 2020, **13**, 2264–2270.