Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Synthesis of pyridine-based covalent organic framework as anode materials for lithium-ion batteries

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Materials

1,3,5-triformylphloroglucinol (Tp), 2,2'-bipyridine-5,5'-diamine (Bpy) were purchased from Jilin Chinese Academy of Sciences-Yanshen Technology Co., Ltd. Other reagents including 1,4-dioxane, mesitylene, N, N-dimethylformamide (DMF), tetrahydrofuran (THF), N-Methylpyrrolidone (NMP), acetic acid, etc. were purchased from Sigma-Aldrich Inc. The electrolyte (1 M $LiPF_6$ in EC/DEC, v:v = 1:1) used in the electrochemical measurements was purchased from DoDoChem None of the reagents mentioned above underwent further purification.

Supporting Figures and Tables

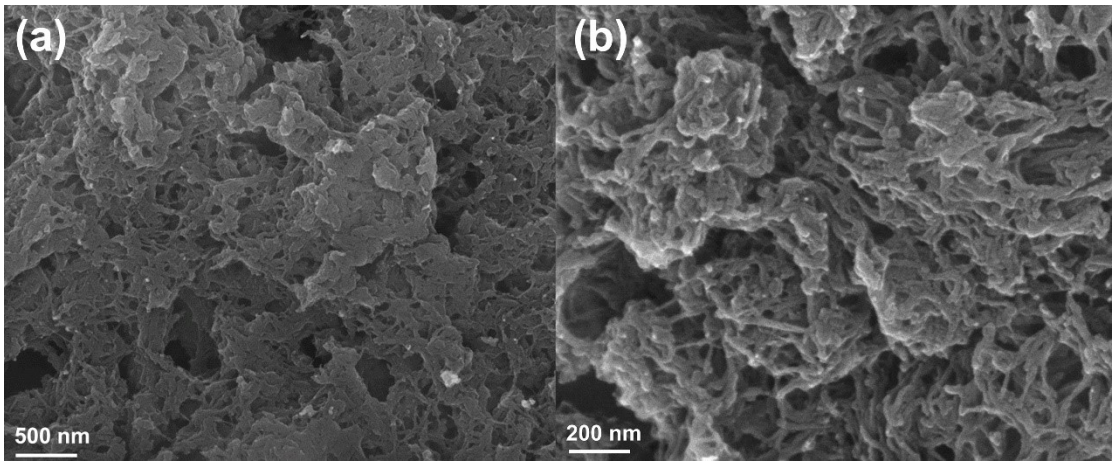

Fig. S1 SEM images of TpBpy before ball milling.

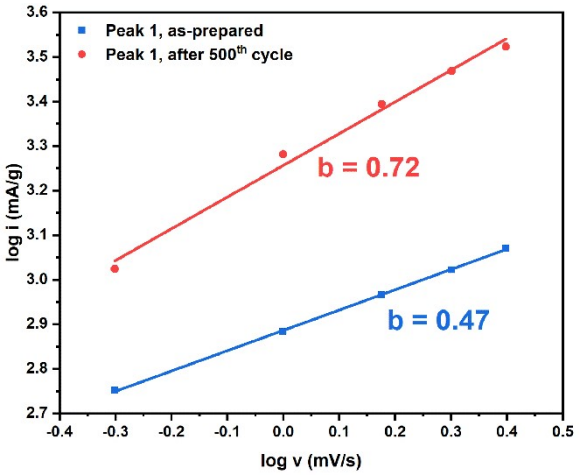

Fig. S2 Plots of log current vs. log scan rate to determine the b values of Peak 1 of TpBpy as-prepared and after the 500th cycle

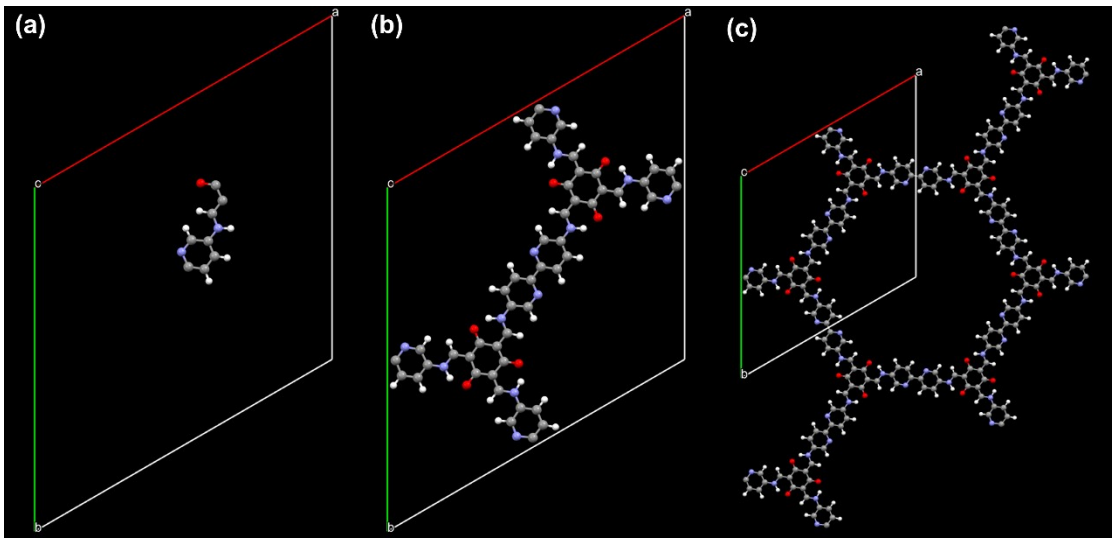

Fig. S3 The (a) asymmetric unit, (b) unit cell, and (c) eclipsed crystal lattice packing of TpBpy.

TpBpy			
Hexagonal, *P*6 a=b=29.00 Å, c=3.57 Å α=β=90°, γ=120°			
C1	0.5167	0.4893	0.4754
C2	0.5709	0.523	0.4751
C3	0.6043	0.5022	0.4751
C4	0.5271	0.4165	0.4753
C5	0.5833	0.4479	0.4753
C6	0.597	0.3745	0.4751
C7	0.6314	0.3539	0.4765
C8	0.6085	0.2978	0.4754
N1	0.4938	0.4347	0.4767
N2	0.6166	0.427	0.4751
O1	0.5583	0.2667	0.4751
H1	0.5861	0.5657	0.4587
H2	0.5083	0.3731	0.4755
H3	0.6471	0.5284	0.4515
H4	0.5541	0.3458	0.4523
H5	0.6592	0.4489	0.46

Table S1 Fractional atomic coordinates for the asymmetric unit of TpBpy.

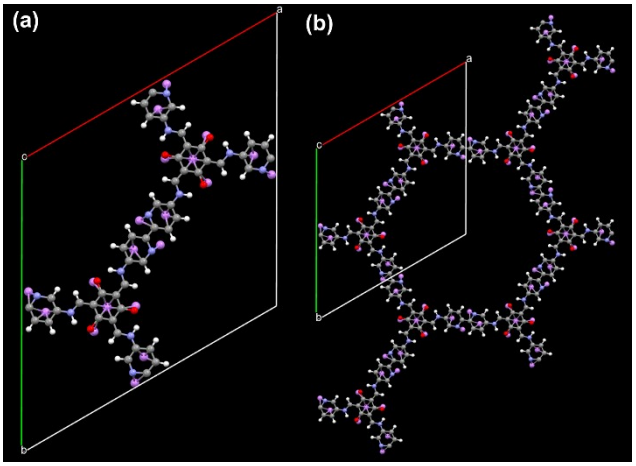

Fig. S4 The (a) unit cell, and (b) eclipsed crystal lattice packing of 20Li-TpBpy.

20Li-TpBpy			
Triclinic, *P*1 a=30.15 Å, b=30.04 Å, c=3.60 Å α=90.02°, β=90.04° γ=120.12°			
C1	0.519986	0.49209	0.174428
C2	0.575398	0.525739	0.174686
C3	0.607094	0.502856	0.173147
C4	0.530412	0.416936	0.149682
C5	0.584579	0.447187	0.149656
C6	0.601869	0.375739	0.149473
C7	0.636593	0.357151	0.144936
C8	0.615102	0.301484	0.124948
C9	0.512595	0.028941	0.14867
C10	0.480078	0.049702	0.125028
C11	0.500265	0.10429	0.164615
C12	0.587333	0.114975	0.174731
C13	0.556219	0.136878	0.173325
C14	0.626919	0.224296	0.174688
C15	0.648341	0.279072	0.147995
C16	0.704388	0.31355	0.125244
C17	0.97603	0.485094	0.172904
C18	0.953309	0.42966	0.150266
C19	0.900611	0.39684	0.174172
C20	0.890067	0.476061	0.173735
C21	0.868153	0.421351	0.150935
C22	0.779952	0.404174	0.149548
C23	0.726333	0.369322	0.144854
C24	0.692392	0.390847	0.124986
C25	0.487462	0.512346	0.149737
C26	0.432477	0.47821	0.125031
C27	0.399462	0.500231	0.14827
C28	0.476092	0.586371	0.174521
C29	0.420741	0.555503	0.174306
C30	0.404471	0.627734	0.174234
C31	0.370425	0.647441	0.158055
C32	0.390029	0.70268	0.124919
C33	0.491283	0.973527	0.173374
C34	0.526234	0.953422	0.164893
C35	0.505189	0.89876	0.148476
C36	0.418575	0.890873	0.174264
C37	0.448552	0.867161	0.125631
C38	0.376204	0.779667	0.149191
C39	0.357456	0.725865	0.147118

C40	0.302827	0.690549	0.150679
C41	0.02972	0.518382	0.1506
C42	0.051659	0.57341	0.174357
C43	0.106447	0.606678	0.149359
C44	0.115824	0.529652	0.173611
C45	0.138418	0.583862	0.151451
C46	0.22702	0.601351	0.151302
C47	0.281642	0.634955	0.173964
C48	0.315509	0.613722	0.15052
N1	0.497065	0.437657	0.164607
N2	0.618444	0.428191	0.148884
N3	0.567504	0.059644	0.167057
N4	0.573704	0.188614	0.174979
N5	0.945054	0.509303	0.164756
N6	0.815506	0.387282	0.145928
N7	0.509865	0.567332	0.174749
N8	0.388862	0.57546	0.174833
N9	0.436588	0.944427	0.174832
N10	0.42834	0.815299	0.145149
N11	0.059846	0.494179	0.14602
N12	0.192373	0.617111	0.174541
O1	0.561754	0.266087	0.124704
O2	0.737954	0.294664	0.173996
O3	0.713059	0.443945	0.124527
O4	0.442367	0.735877	0.124576
O5	0.270054	0.712311	0.17457
O6	0.29569	0.561684	0.174533
H1	0.593441	0.567874	0.149459
H2	0.509751	0.375786	0.192133
H3	0.647862	0.526481	0.144416
H4	0.561225	0.348736	0.194605
H5	0.65809	0.451138	0.141737
H6	0.438124	0.025439	0.099483
H7	0.62927	0.1391	0.199291
H8	0.477661	0.123388	0.140801
H9	0.652853	0.209148	0.195093
H10	0.551408	0.204582	0.149019
H11	0.978904	0.414343	0.144453
H12	0.866012	0.493924	0.197082
H13	0.882726	0.354757	0.149217
H14	0.793812	0.444844	0.199317
H15	0.799088	0.347755	0.147164
H16	0.414564	0.436136	0.149298

H17	0.494063	0.628347	0.198558
H18	0.358729	0.4739	0.149179
H19	0.444202	0.653635	0.141969
H20	0.348452	0.55062	0.14938
H21	0.567835	0.980452	0.149463
H22	0.376684	0.866778	0.14932
H23	0.52711	0.879573	0.141819
H24	0.351157	0.795017	0.198587
H25	0.450809	0.798663	0.097373
H26	0.027771	0.591264	0.174512
H27	0.139918	0.511919	0.197205
H28	0.121285	0.64731	0.149328
H29	0.212193	0.56104	0.199332
H30	0.206392	0.656736	0.125241
Li1	0.447938	0.723455	0.603296
Li2	0.284164	0.728468	0.652798
Li3	0.281232	0.557915	0.65354
Li4	0.728991	0.444767	0.604443
Li5	0.723995	0.280806	0.652595
Li6	0.561306	0.278337	0.605098
Li7	0.543811	0.563441	0.648841
Li8	0.461103	0.438971	0.647402
Li9	0.567373	0.02754	0.649179
Li10	0.444482	0.983657	0.647719
Li11	0.026127	0.46255	0.645288
Li12	0.980384	0.543364	0.648997
Li13	0.479813	0.912498	0.646049
Li14	0.335525	0.670523	0.64724
Li15	0.094395	0.566671	0.646543
Li16	0.438798	0.52618	0.647955
Li17	0.563751	0.472124	0.649702
Li18	0.670662	0.335002	0.643041
Li19	0.909486	0.442175	0.649579
Li20	0.533339	0.096573	0.651439

Table S2 Fractional atomic coordinates for the unit cell of 20Li-TpBpy.

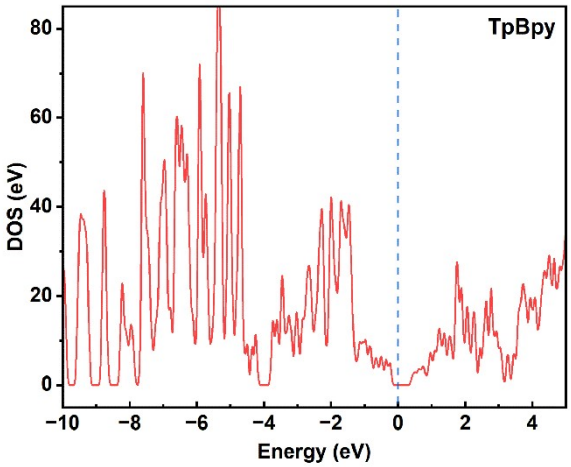

Fig. S5 The electron DOS of TpBpy.

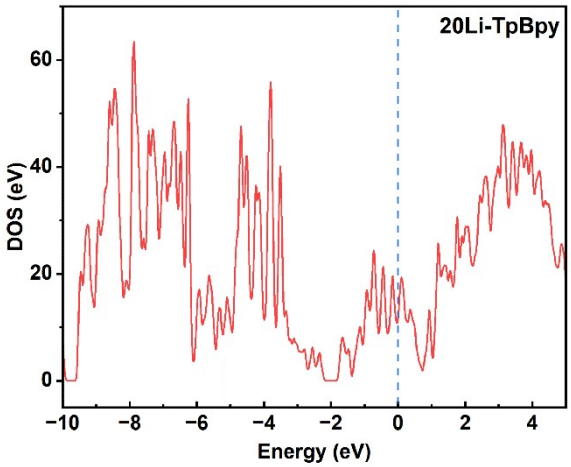

Fig. S6 The electron DOS of 20Li-TpBpy.