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


# Supporting Information

## Hexaazatriphenylene derivatives/GO composites as organic cathodes for lithium ion batteries

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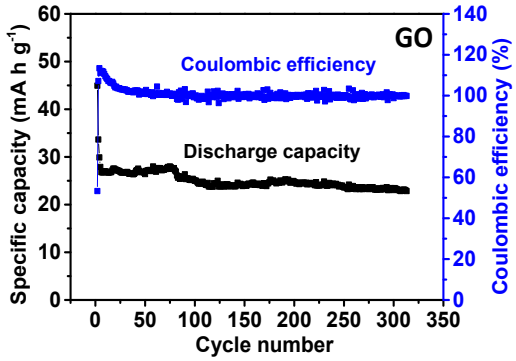



**Figure S1** Cycle performances at 50 mA/g for blank GO. (GO: PVDF = 5:1)

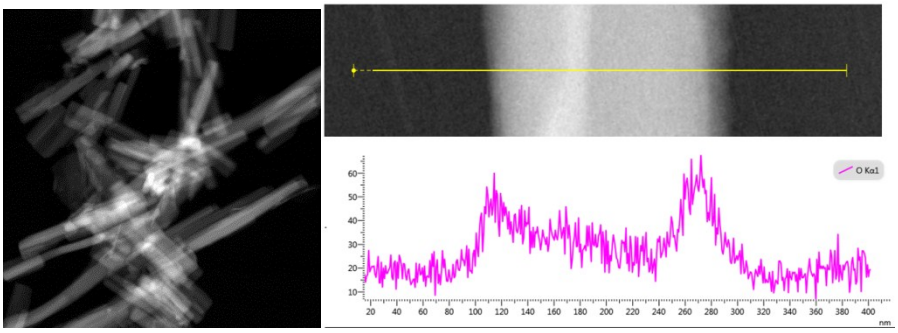



**Figure S2** STEM image (GO: white color, HATN nanorod: deep gray color) and EDX line-scan profile of O element of HATN/GO nano-rod, condition: HATN (20 mg), GO (16 mg), sonicated in 10 mL toluene for 6 h.

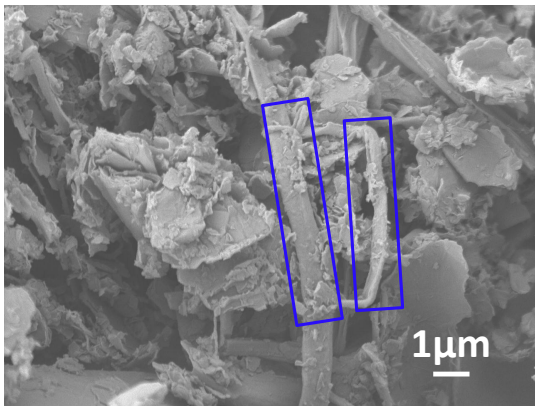



**Figure S3** SEM image of HATN/GO after dissolving the HATN nanorod in $CHCl_3$. The HATN/GO composite was soaked in $CHCl_3$ and shaken until all the HATN was dissolved. Residual GO demonstrates empty tube-like structure (blue box).

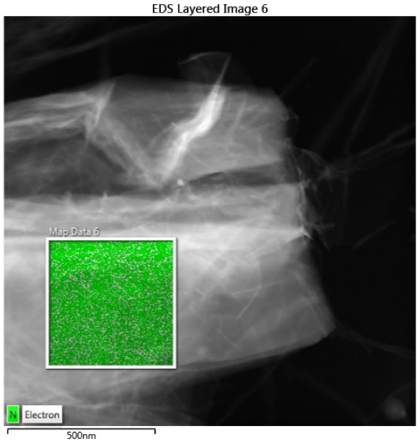



**Figure S4** STEM image and EDX mapping profile of N element of HATNTA/GO composite, condition: HATNTA (20 mg), GO (16 mg), sonicated in 10 mL ethanol for 6 h.

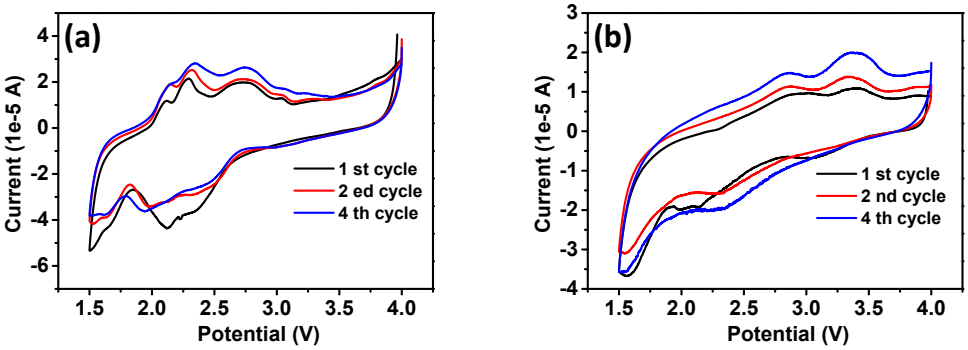



**Figure S5** CV curves of the composites of (a) HATN/GO and (b) HATNTA/GO measured with scan rate of 0.2 mV $S^{-1}$.

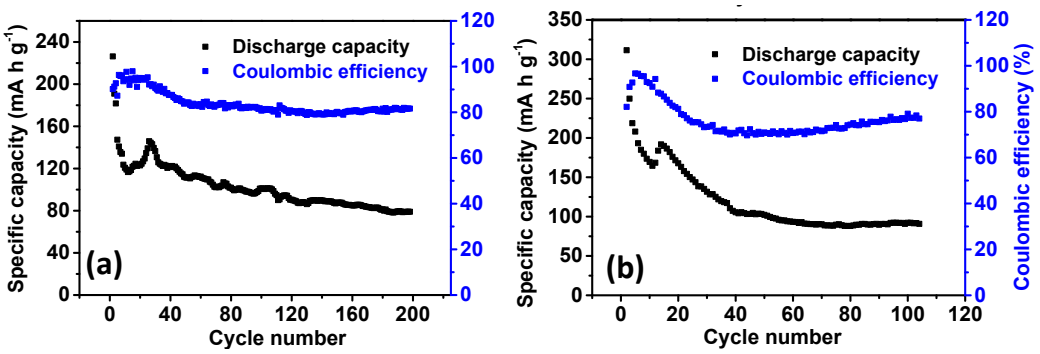



**Figure S6** Cycle performances at 50 mA/g for mixtures of (a) HATN and GO, and (b) HATNTA and GO (both without nanocomposites prefabrication using sonication method). Condition: HATN or HATNTA: GO:PVDF = 5:4:1, shaken in vortex for 12 h.

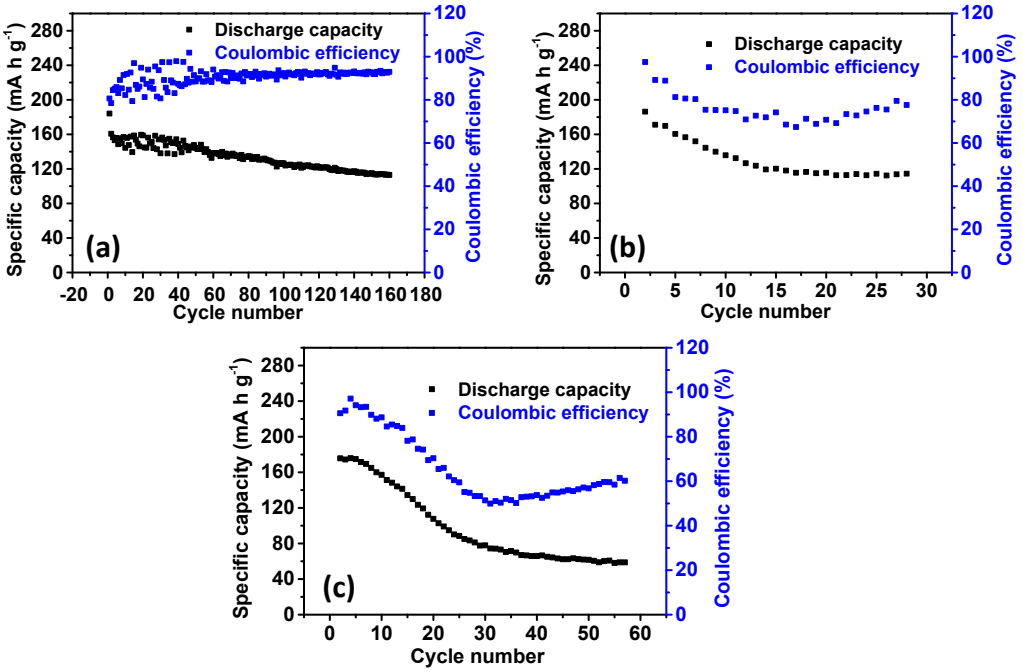



**Figure S7** Cycle performances of HATN at 50 mA/g with different conductive carbon sources(a) RGO or (b) CNT with diameter 50 nm or (c) VGCF under the same condition with GO.

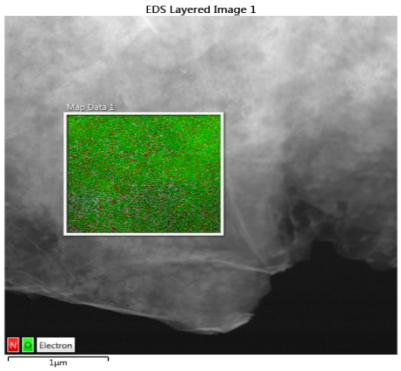



**Figure S8** STEM image and EDX mapping profile of N and O element of HATNTA/GO composite after cycling test.

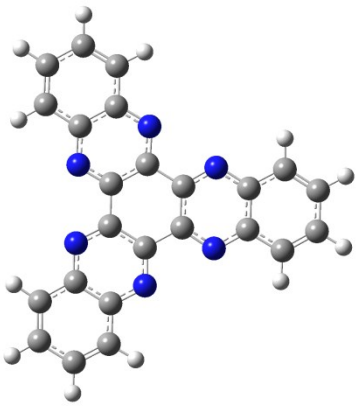
**Table S1 A** comparison of HATN based electrodes.

| Materials | Active Material/Conductive Material/PVDF | Electrolyte | Capacity ( mA h/g) | Ref |
|---|---|---|---|---|
| HATN/GO | 5:4:1 | $LiPF_6$/EC+DMC | 410 at 50 mA/g | This work |
| HATN/RGO | 6:3:1 | LiTFSI-DOL/DME | ~220 at 400mA/g | 22 |
| Poly-HATN | 6:3:2 | $LiPF_6$/EC+DMC | 147 at 100mA/g | 23 |
| HATN | 5:4:1 | Solid one | ~250 at 0.2C and 323 K | 21 |

**Computational Details**

The calculations were carried out by performing DFT by use of the B3PW91functional with the 6-31G (d) basis set as implemented in Gaussian 09 program package. Vibrational frequency calculations, from which the zero-point energies were derived, have been performed for each optimized structure at the same level to identify the natures of all the stationary points.

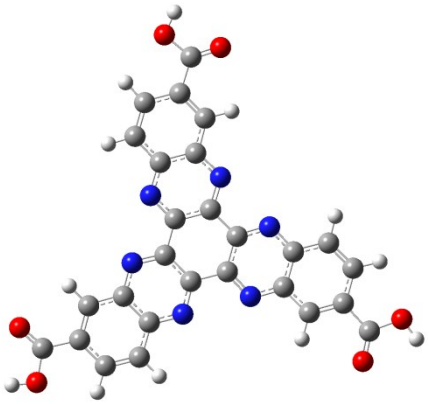
Cartesian coordinates for the optimized geometries



HATN

| | | | |
|---|---|---|---|
| C | -0.05370100 | -1.45764100 | -0.00008800 |
| C | -1.27805800 | -0.70205000 | -0.00007000 |
| C | 1.24741700 | -0.75612500 | -0.00012300 |
| C | -1.23508300 | 0.77539700 | -0.00006300 |
| C | 0.03130400 | 1.45819500 | -0.00012000 |
| C | 1.28928500 | 0.68203600 | -0.00013400 |
| N | -2.38070500 | 1.43876600 | 0.00005000 |
| N | 0.10641100 | 2.77989900 | -0.00014700 |
| N | -2.46039200 | -1.29756000 | -0.00000400 |
| N | -0.05579300 | -2.78153300 | -0.00003300 |
| N | 2.35443900 | -1.48209600 | -0.00005600 |
| N | 2.43673700 | 1.34236100 | -0.00008100 |
| C | -1.25691200 | -3.40323700 | 0.00002500 |
| C | -1.31331700 | -4.82343000 | 0.00007500 |
| C | -2.47741500 | -2.64987000 | 0.00003500 |
| C | -2.53270200 | -5.45912600 | 0.00012300 |
| H | -0.37523100 | -5.36963800 | 0.00006900 |
| C | -3.72154800 | -3.33707000 | 0.00008900 |
| C | -3.74303600 | -4.71202500 | 0.00012800 |
| H | -2.57907300 | -6.54469000 | 0.00015900 |
| H | -4.63038500 | -2.74347900 | 0.00009100 |
| C | -2.31890400 | 2.78977000 | 0.00005200 |
| C | -3.52079100 | 3.54845700 | 0.00015600 |
| C | -1.05641000 | 3.47052100 | -0.00007900 |
| C | -3.46204900 | 4.92231500 | 0.00013300 |
| H | -4.46275300 | 3.00894600 | 0.00025700 |
| C | -1.02994100 | 4.89156500 | -0.00010100 |
| C | -2.21009200 | 5.59738300 | 0.00000300 |
| H | -4.37919600 | 5.50492700 | 0.00021900 |
| H | -0.06159300 | 5.38212500 | -0.00019900 |
| C | 3.53398400 | -0.82045300 | -0.00001500 |
| C | 3.57574100 | 0.61322100 | -0.00002900 |
| C | 4.75125500 | -1.55410800 | 0.00001700 |
| C | 4.83377500 | 1.27469600 | 0.00001600 |
| C | 5.95265400 | -0.88504000 | 0.00006100 |
| H | 4.69180100 | -2.63799100 | 0.00002300 |
| C | 5.99408900 | 0.53672100 | 0.00006300 |
| H | 4.83760100 | 2.36021800 | 0.00000900 |

| | | | |
|---|---|---|---|
| H | 6.95729800 | 1.03955400 | 0.00009700 |
| H | 6.88493600 | -1.44310800 | 0.00009700 |
| H | -4.69261000 | -5.24013800 | 0.00016700 |
| H | -2.19295600 | 6.68379900 | -0.00001900 |



HATNTA

| | | | |
|---|---|---|---|
| C | 1.03330900 | -1.02986900 | -0.00015600 |
| C | 1.41441700 | 0.35816900 | 0.00016500 |
| C | -0.39683300 | -1.40435100 | -0.00019400 |
| C | 0.37506200 | 1.40943300 | 0.00012000 |
| C | -1.01761300 | 1.04554000 | -0.00004800 |
| C | -1.40832300 | -0.38020200 | -0.00003800 |
| N | 0.76078500 | 2.67478800 | 0.00017100 |
| N | -1.97471400 | 1.95947800 | -0.00023200 |
| N | 2.68442000 | 0.73018700 | 0.00047500 |
| N | 1.93637400 | -1.99654600 | -0.00034100 |
| N | -0.70977300 | -2.69017300 | -0.00031400 |
| N | -2.69701700 | -0.67888000 | 0.00011400 |
| C | 3.23909400 | -1.63026900 | -0.00013300 |
| C | 4.24476600 | -2.62947900 | -0.00033100 |
| C | 3.61875900 | -0.24780800 | 0.00036300 |
| C | 5.57633100 | -2.26637200 | -0.00000800 |
| H | 3.95452400 | -3.67428000 | -0.00074400 |
| C | 4.99771200 | 0.09665300 | 0.00072300 |
| C | 5.95289300 | -0.88969500 | 0.00054000 |
| H | 5.25928300 | 1.14982900 | 0.00112100 |
| C | -0.20767200 | 3.61991000 | 0.00004800 |
| C | 0.15492200 | 4.99040800 | 0.00010900 |
| C | -1.59481700 | 3.25759300 | -0.00018800 |
| C | -0.82521500 | 5.96212300 | -0.00008000 |
| H | 1.20486000 | 5.26147000 | 0.00033600 |
| C | -2.58249500 | 4.27965200 | -0.00038500 |
| C | -2.20579100 | 5.59999800 | -0.00033700 |
| H | -3.62538500 | 3.97969600 | -0.00057000 |
| C | -2.02395200 | -3.01026100 | -0.00021900 |
| C | -3.03126400 | -1.99013500 | 0.00005200 |
| C | -2.41540900 | -4.37659400 | -0.00035900 |
| C | -4.39946700 | -2.36129200 | 0.00023300 |
| C | -3.74728100 | -4.71050000 | -0.00020100 |

| | | | |
|---|---|---|---|
| H | -1.63431700 | -5.12992000 | -0.00059000 |
| C | -4.75111100 | -3.69590600 | 0.00011200 |
| H | -5.15908400 | -1.58744900 | 0.00049100 |
| H | -4.05302500 | -5.75038400 | -0.00029900 |
| H | 7.00635300 | -0.63474700 | 0.00080200 |
| H | -2.95332100 | 6.38485100 | -0.00048900 |
| C | -6.20382400 | -4.03058400 | 0.00030900 |
| O | -7.10427800 | -3.21722200 | 0.00057700 |
| O | -6.43387900 | -5.36792700 | 0.00013600 |
| H | -7.40370000 | -5.47074300 | 0.00036700 |
| C | 6.59333500 | -3.35635300 | -0.00021900 |
| O | 6.34032400 | -4.54307000 | -0.00091100 |
| O | 7.86614000 | -2.88564400 | 0.00045400 |
| H | 8.44086300 | -3.67355900 | 0.00016600 |
| C | -0.38942600 | 7.38775900 | -0.00002500 |
| O | 0.76493800 | 7.76161800 | 0.00021000 |
| O | -1.43325300 | 8.25490600 | -0.00029800 |
| H | -1.03816100 | 9.14655300 | -0.00016900 |