

Supporting Information

2D conductive MOF with sufficient redox sites: reduced graphene oxide/Cu-benzenehexathiolate composites as high capacity anode materials for lithium-ion battery

Chunfeng Meng,^a Pinfei Hu,^b Hantao Chen,^b Yueji Cai,^b Hu Zhou,^a Zehong Jiang,^b Xiang Zhu,^c Zeyu Liu,^b Chengyin Wang,^d and Aihua Yuan^{* b}

^a School of Material Science and Technology, Jiangsu University of Science and Technology, Zhenjiang, Jiangsu 212003, P. R. China

^b School of Environmental and Chemical Engineering, Jiangsu University of Science and Technology, Zhenjiang, Jiangsu 212003, P. R. China

^c Suzhou Research Institute, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou 730000, P. R. China

^d School of Chemical and Chemistry Engineering, Yangzhou University, Yangzhou, Jiangsu 225002, P. R. China

E-mail: aihua.yuan@just.edu.cn

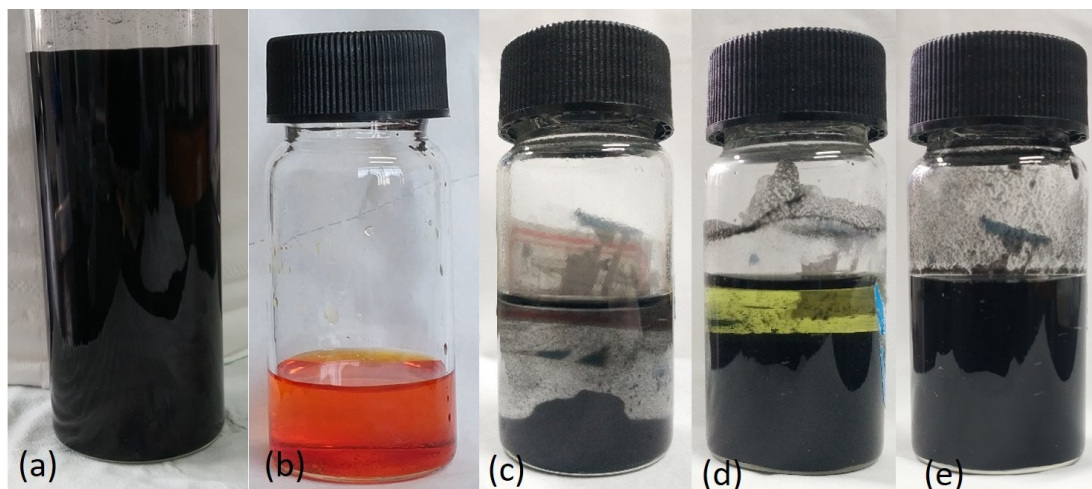


Figure S1. (a) Optical images of rGO dispersion after prepared for a week, (b) BHT solution in DMF, (c) as-prepared Cu-BHT in DMF, (d) rGO/Cu-BHT 1:1 composite in DMF, 10 min after reaction, (e) rGO dispersion and Cu-BHT solid after sonication and rest for 1 hour.

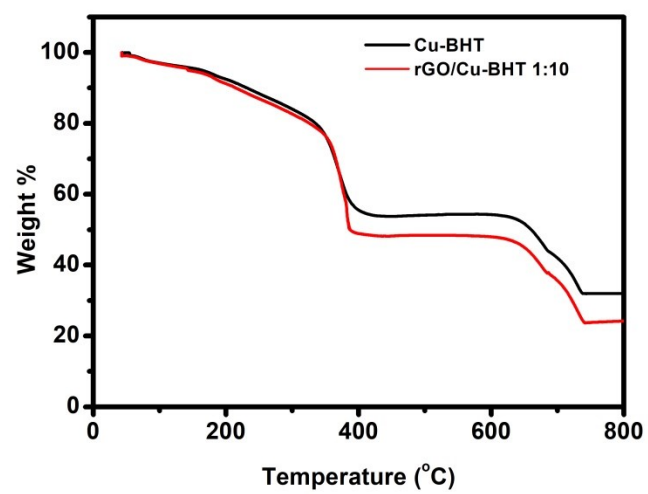


Figure S2. Thermogravimetry study of the Cu-BHT and rGO/Cu-BHT 1:10, in air.

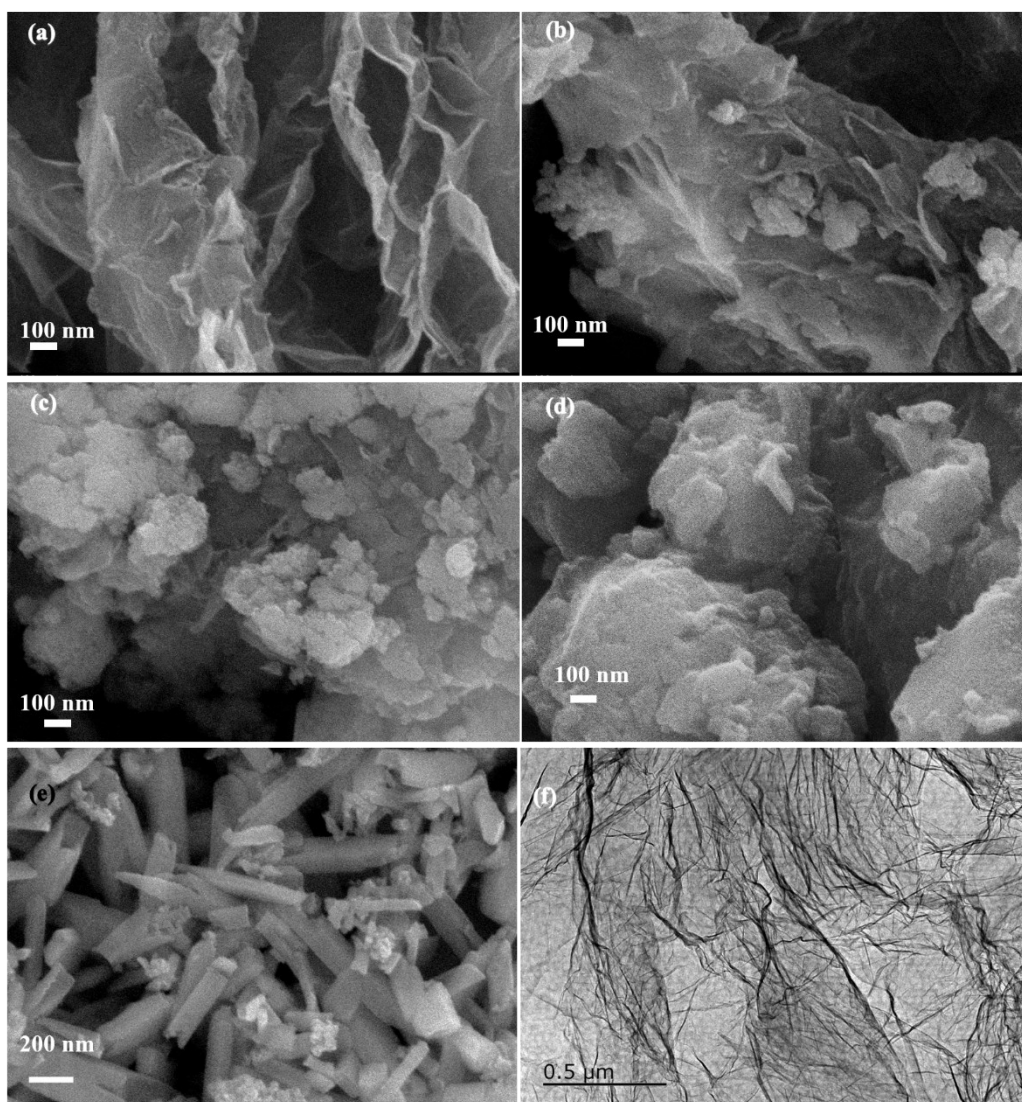


Figure S3. (a, b, c, d, e) FESEM image of rGO/Cu-BHT 3:1, 1:3, 1:10, pristine amorphous Cu-BHT, semicrystalline Cu-BHT; (f) TEM image reduced graphene oxide.

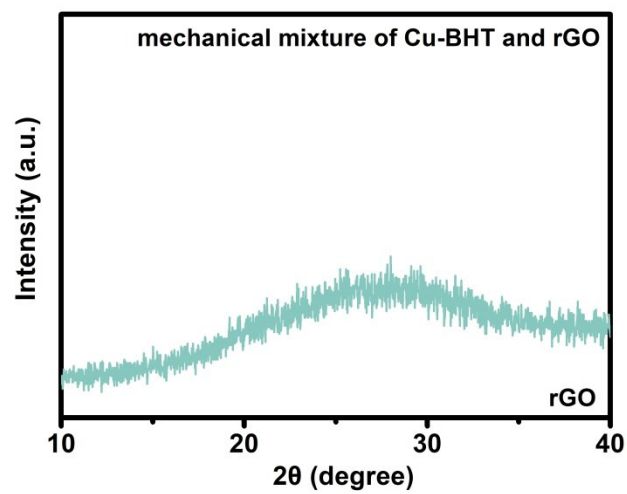


Figure S4. The XRD spectra of the rGO and Cu-BHT mechanical mixture, with a mass ratio of 1:1.

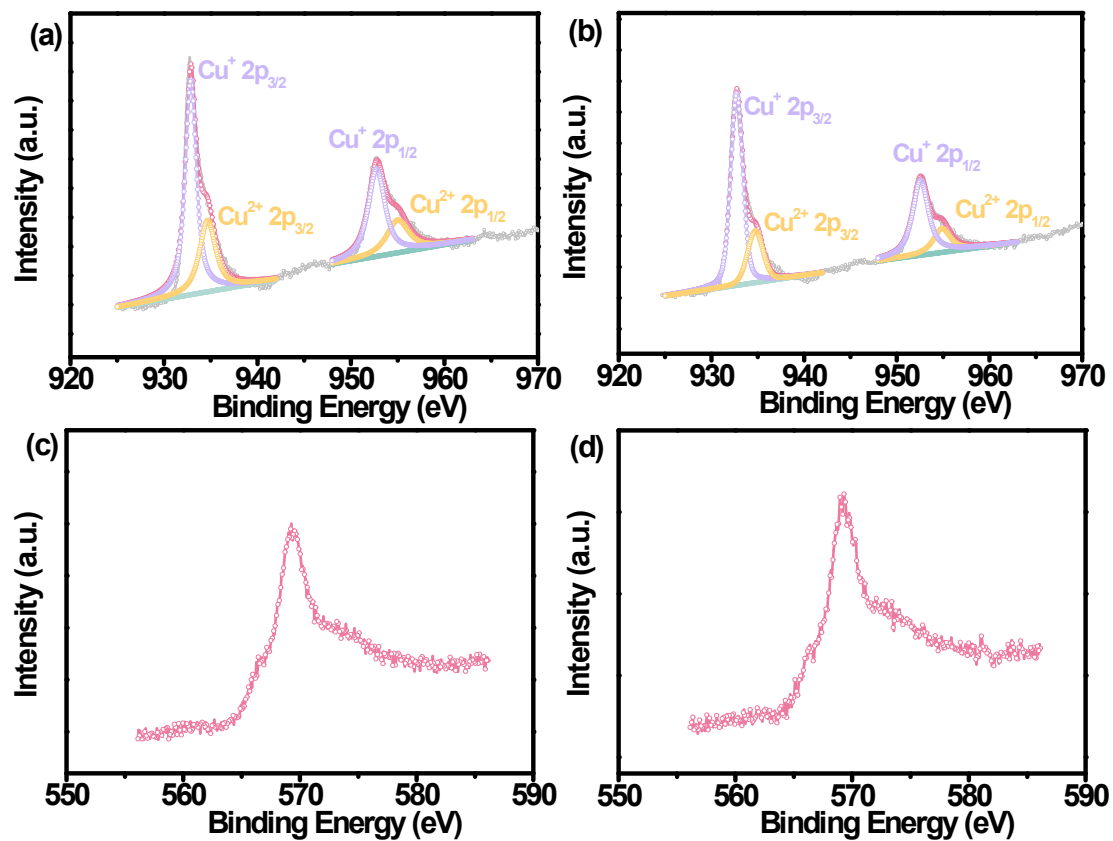


Figure S5. The high-resolution Cu 2p spectra of (a) Cu-BHT and (b) rGO/Cu-BHT 1:1; Cu LMM spectra of (c) Cu-BHT and (d) rGO/Cu-BHT 1:1.

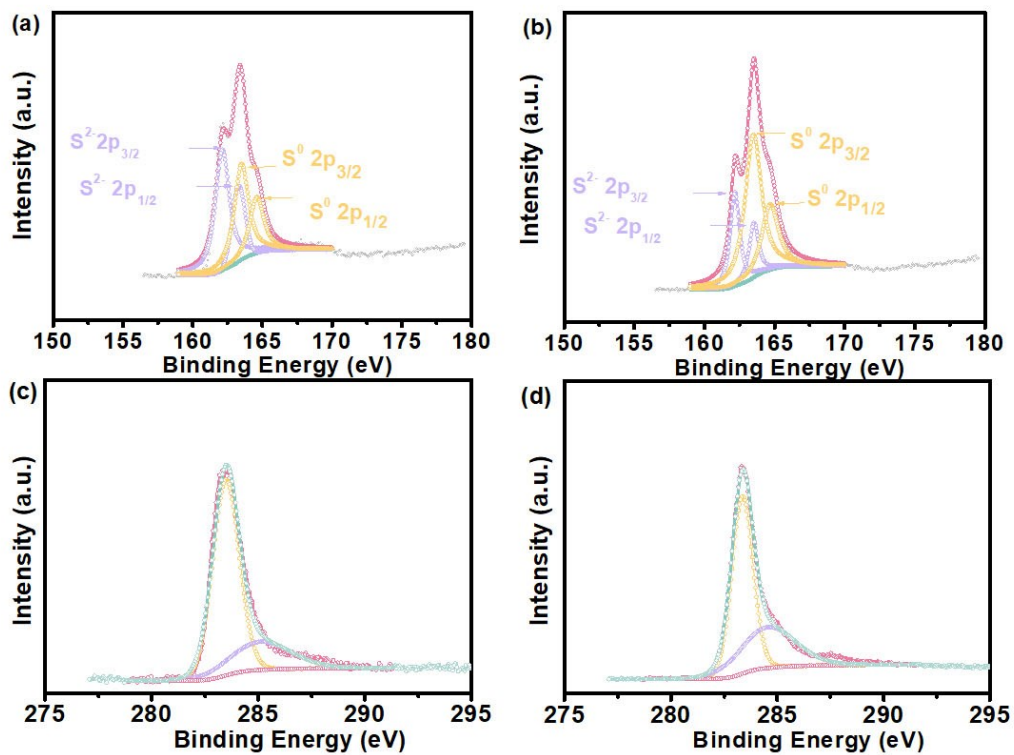


Figure S6. The high-resolution S 2p and C 1s spectra of Cu-BHT (a&c) and rGO/Cu-BHT 1:1(b&d).

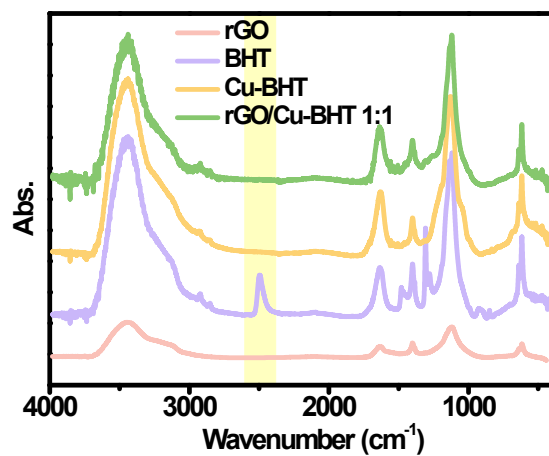


Figure S7. FTIR spectra of Cu-BHT, rGO/Cu-BHT, BHT and rGO.

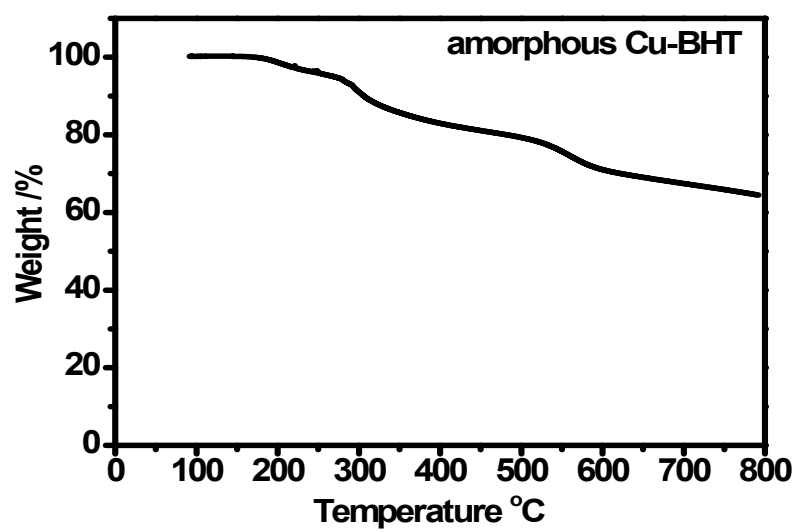


Figure S8. The thermogravimetric curve of Cu-BHT.

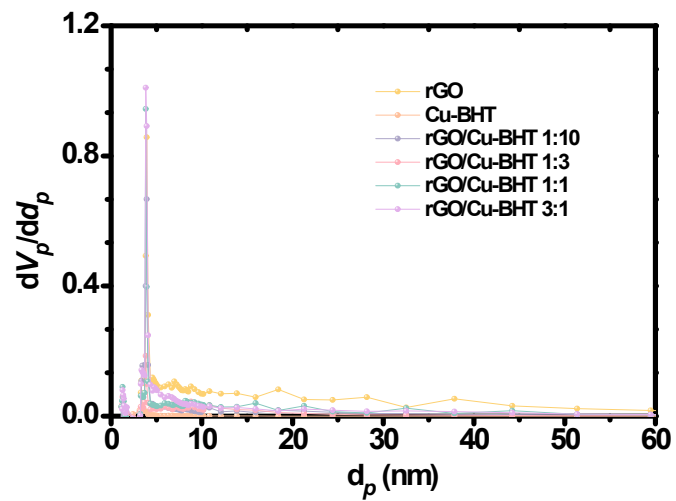


Figure S9. The total pore volumes of reduced graphene oxide, rGO/Cu-BHT (3:1, 1:1, 1:3, 1:10), and pristine Cu-BHT.

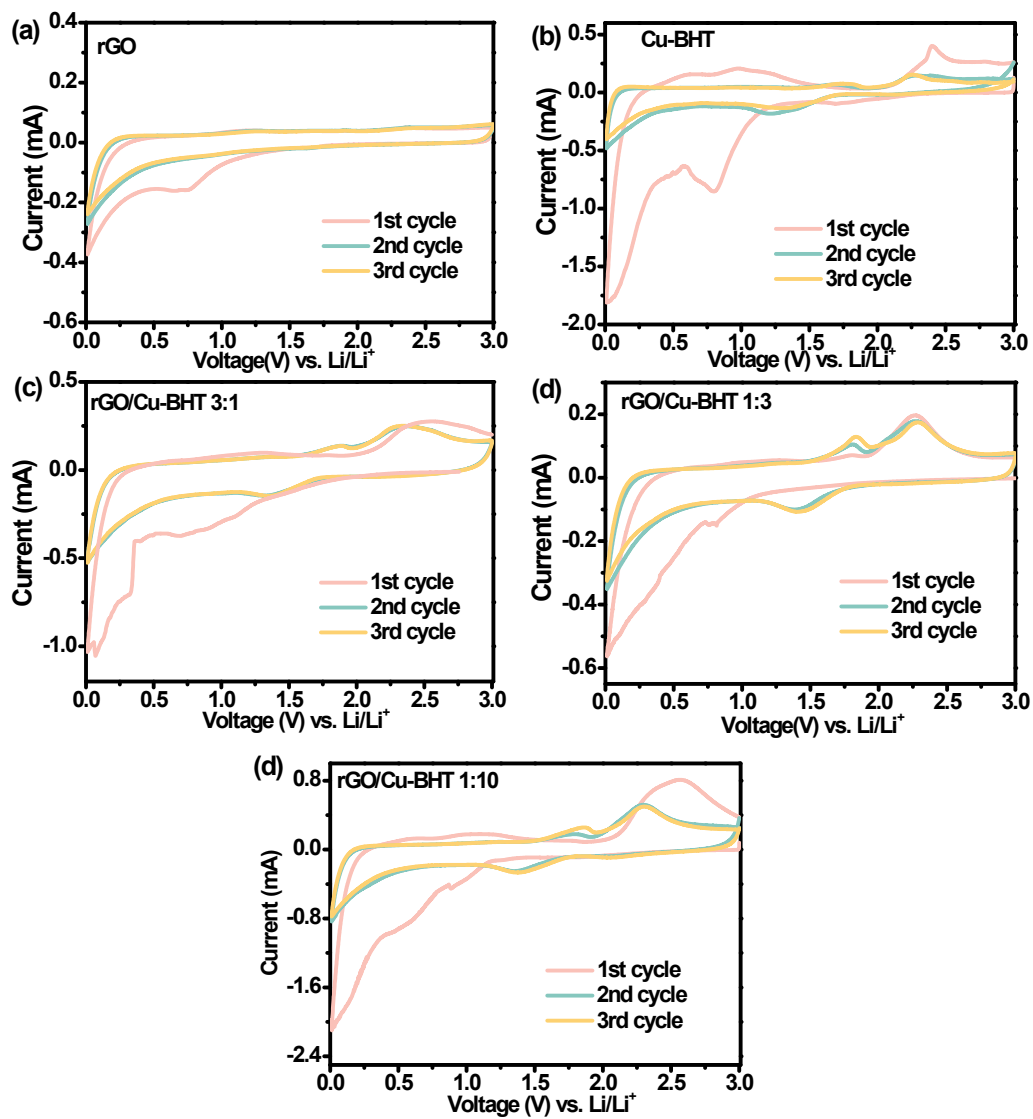


Figure S10. The first three CV curves of (a) reduced graphene oxide, (b) pristine Cu-BHT, (c, d, e) rGO/Cu-BHT (3:1, 1:3, 1:10).

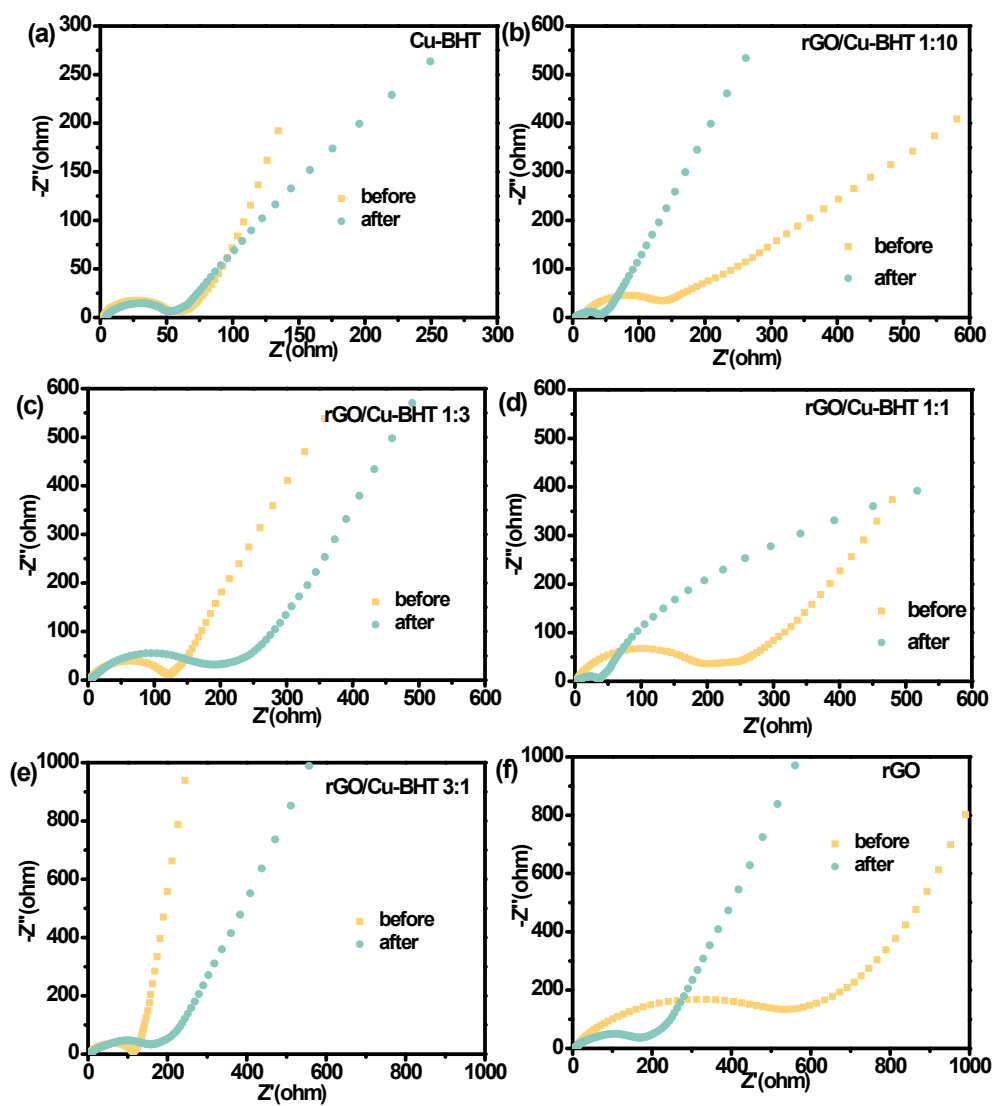


Figure S11. Impedance spectra of (a) Cu-BHT, (b-e) rGO/Cu-BHT (1:10, 1:3, 1:1, 3:1), and (f) rGO.

Figure S12. The plot of Z' vs. the reciprocal root square of the low angular frequencies ($\omega^{-1/2}$).

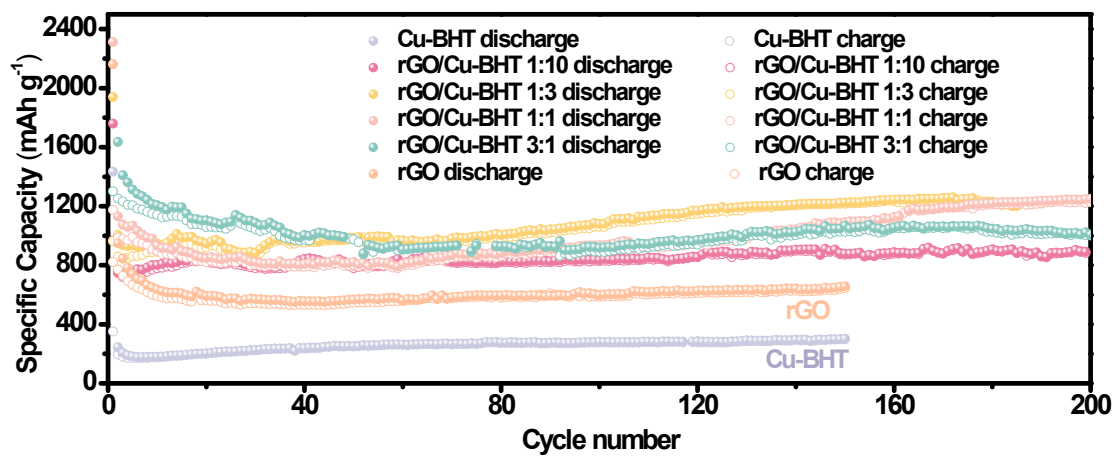


Figure S13. Cycle performance of rGO/Cu-BHT composites at a current density of 100 mA g⁻¹.

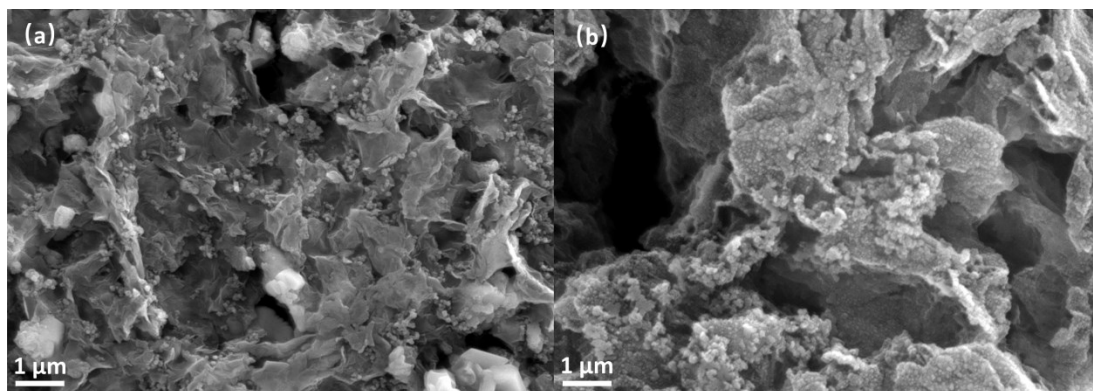


Figure S14. The morphology of rGO/Cu-BHT 1:1, (a) before cycle and (b) after 100 cycles.

Figure S15. Rate performance of (a) amorphous Cu-BHT and (b) rGO/Cu-BHT 1:10.

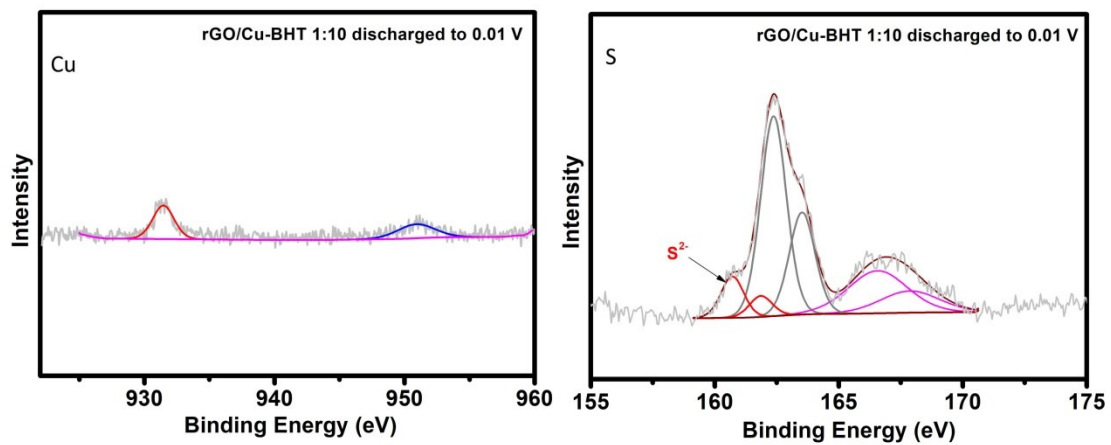


Figure S16. XPS spectrum of discharged Cu-BHT, Cu 2p (left) and S 2p (right).

Table S1. Diffusion coefficients of Cu-BHT based compounds

Sample	Slope (Before cycle)	D_{Li^+} (Before cycle) $cm^2 s^{-1}$	Slope (After cycle)	D_{Li^+} (After cycle) $cm^2 s^{-1}$
Cu-BHT	1046.07	1.32×10^{-15}	894.66	1.80×10^{-15}
1:10	258.18	2.16×10^{-14}	44.29	7.34×10^{-13}
1:3	80.87	2.20×10^{-13}	113.47	1.12×10^{-13}
1:1	71.07	2.15×10^{-13}	34.53	1.21×10^{-12}
3:1	21.49	3.10×10^{-12}	84.89	2.00×10^{-13}
rGO	41.40	1.15×10^{-12}	79.29	3.14×10^{-13}

Contribution calculation of rGO and Cu-BHT in rGO/CuBHT composites

Since the capacity of rGO went steady to 545.2 mAh g⁻¹, so the capacity of rGO was treated as a constant. The capacities of rGO/Cu-BHT (3:1, 1:1, 1:3, 1:10) composites at 100 mA g⁻¹ were listed in the second column in the following Table S2.

The specific capacity contribution of rGO in rGO/CuBHT 3:1 = $3/(3+1) \times 545.2 \text{ mAh g}^{-1} / 1008.9 \text{ mAh g}^{-1} = 40.5\%$, and hence the contribution of Cu-BHT = $1 - 40.5\% = 59.5\%$.

The specific capacity contribution of rGO in rGO/CuBHT 1:1 = $1/(1+1) \times 545.2 \text{ mAh g}^{-1} / 1249.5 \text{ mAh g}^{-1} = 21.8\%$, and hence the contribution of Cu-BHT = $1 - 21.8\% = 78.2\%$.

The specific capacity contribution of rGO in rGO/CuBHT 1:3 = $1/(1+3) \times 545.2 \text{ mAh g}^{-1} / 1218.5 \text{ mAh g}^{-1} = 11.2\%$, and hence the contribution of Cu-BHT = $1 - 11.2\% = 88.8\%$.

The specific capacity contribution of rGO in rGO/CuBHT 1:10 = $1/(1+10) \times 545.2 \text{ mAh g}^{-1} / 891.1 \text{ mAh g}^{-1} = 5.5\%$, and hence the contribution of Cu-BHT = $1 - 5.5\% = 94.5\%$.

Table S2. Weight ratios and capacity contributions of rGO and Cu-BHT in composites

Sample	Specific capacity, mAh g ⁻¹	Weight ratio of rGO	Capacity contribution of rGO	Weight ratio of Cu-BHT	Capacity contribution of Cu-BHT
rGO/CuBHT 3:1,	1008.9	75%	40.5%	25%	59.5%.
rGO/CuBHT 1:1	1249.5	50%	21.8%	50%	78.2%
rGO/CuBHT 1:3	1218.5	25%	11.2%	75%	88.8%
rGO/CuBHT 1:10	891.1	9.1%	5.5%	90.9%	94.5%