Supporting information

Understanding the degradation mechanism of rechargeable lithium/sulfur cells: a comprehensive study of the sulfur-graphene oxide cathode after discharge/charge cycling

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Figure S1. Total electron yield (TEY) S K-edge NEXAFS spectra of elemental S (S₈) and S-GO.

S2. S K-edge TEY spectra of pure LiTFSI



Figure S2. TEY NEXAFS spectra of S K-edge of pure LiTFSI.

S3. O K-edge TEY spectra of the cathode materials before and after cycling

For the S-GO cathode materials with o cycle, several absorption features can be observed. The peak at 531.1 eV and 533.7 eV are assigned as the O is transition to carboxyl π^* and epoxide π^* , respectively.¹⁻³ It should be mentioned that the 533.7 eV peak can also be attributed the O is transition to the π^* orbital of C=O in Li₂CO₃.⁴ The peak around 537.1 eV is due to the O is transition to S-O σ^* , while the feature at 539.4 eV should be the contribution of O is transition to C-O σ^* .¹ After cycling, the ratio of the peaks at 537.1 eV and 539.4 eV increases, implying the formation of possible lithium sulfite and lithium sulfate species on the cathode interface. The damping of the feature at 531.1 eV shows the strong interaction between Li atoms and carboxyl. In addition, the intensification of the 533.7 eV feature after 100 cycles proves the formation of Li₂CO₃ on the S-GO cathode surface.



Figure S₃. TEY NEXAFS of O K-edge of the S-GO cathode materials at different discharge/charge cycles. All electrodes were examined in the fully charged states.

S4. TFY signals of S K-edge and C K-edge absorption spectra of S-GO cathode



Figure S4. (a) S K-edge and (b) C K-edge absorption spectra of S-GO cathode materials measured with TFY mode.

REFERENCES

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