Supporting Information

Direct Impregnation of SeS_2 into MOFs-derived 3D Nanoporous Co-N-C Architecture Towards Superior Rechargeable Lithium Batteries

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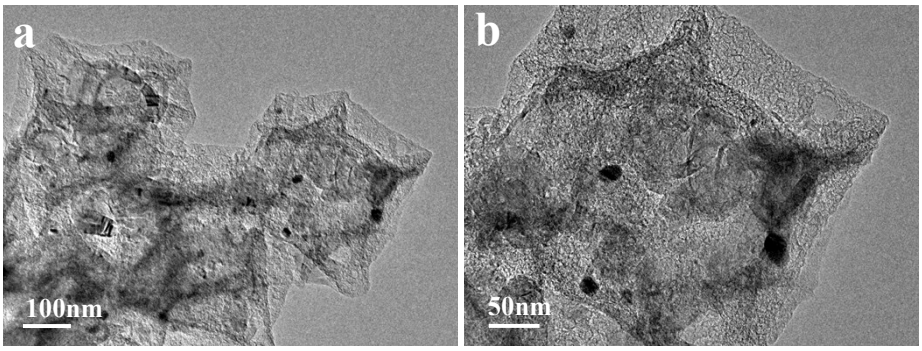


Figure S1. TEM images of Co-N-C.

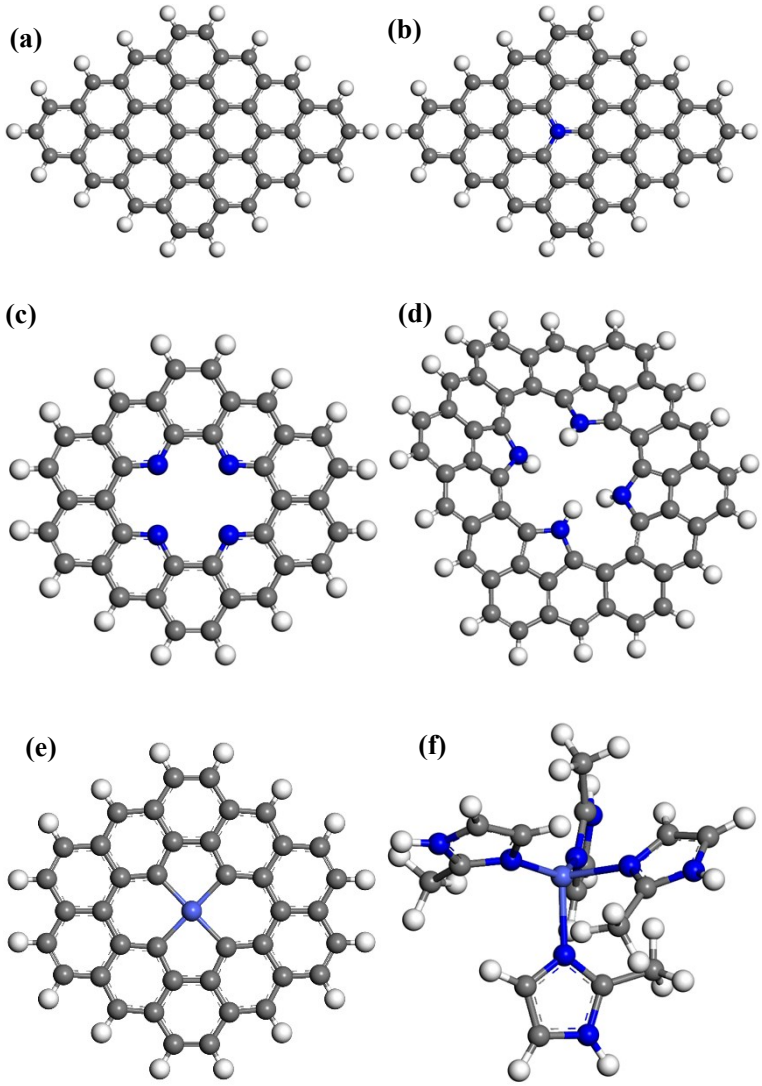
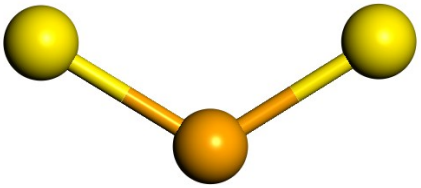


Figure S2. Adsorption host models used to determine the active binding sites for SeS_2 (a) graphene, (b) Graphic N, (c) Pyridine N, (d) Pyrrole N, (e) Graphic Co, (f) Co(2-Methylimidazole)$_4$ which stand for Co-N-C MOF. The white, grey, blue, light blue balls represent H, C, N, Co atoms, respectively.



SeS_2

Figure S3. DFT optimized adsorption structures of SeS_2.

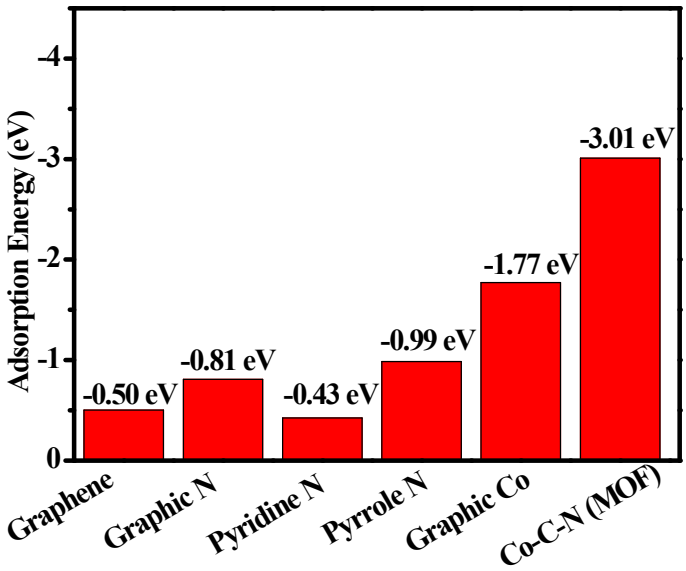


Figure S4. Predicted Adsorption energy of SeS_2 adsorbed on graphene, N-doped graphene, Co-doped graphene and Co-N-C host, respectively.

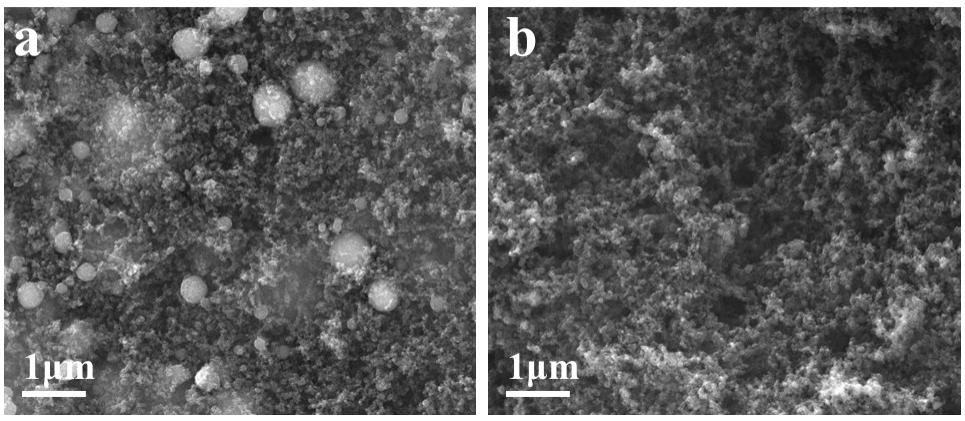


Figure S5. SEM images of (a) SP-Co/SeS_2 and (b) SP/SeS_2.

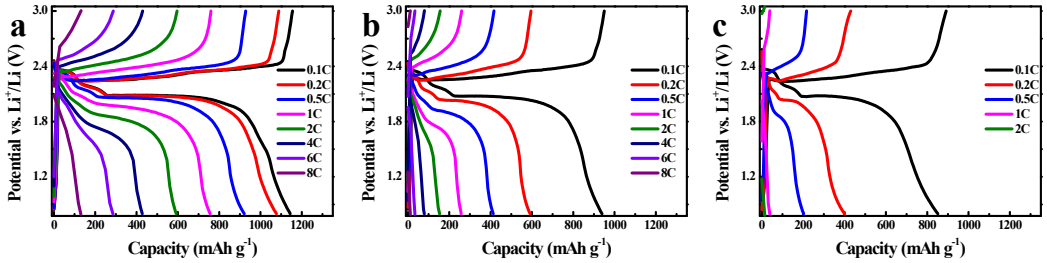


Figure S6. The voltage profiles of (a) Co-N-C/SeS_2, (b) SP-Co/SeS_2, and (c) SP/SeS_2 at various current densities.

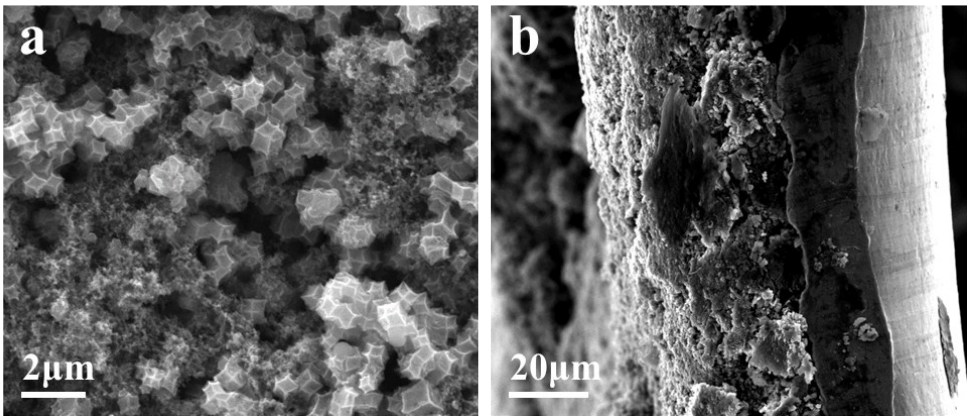


Figure S7. The (a) top view and (b) cross-section SEM images of Co-N-C/SeS_2.

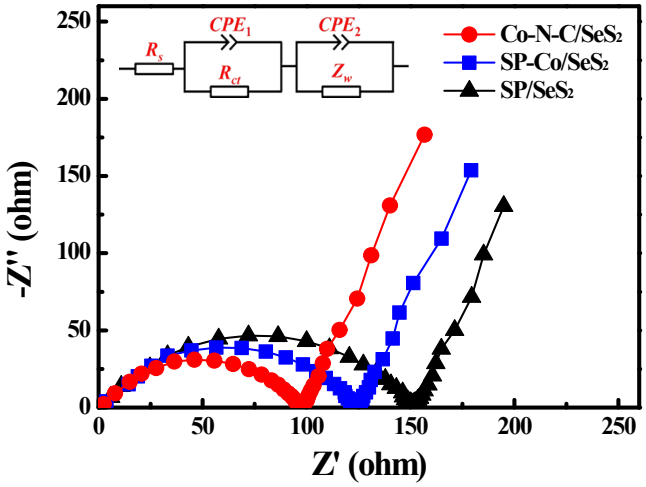


Figure S8. EIS spectra of the SP/SeS_2, SP-Co/SeS_2 and Co-N-C/SeS_2 cathodes before cycling.

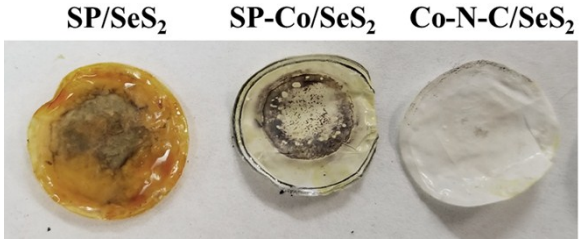


Figure S9. The digital photos of the separators disassembled from cycled coin cells of different groups.

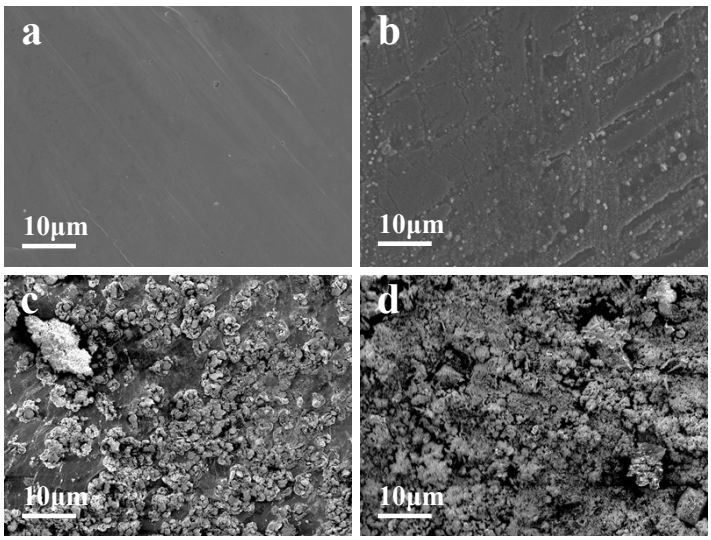


Figure S10. SEM images of (a) fresh Li foil, cycled Li foil in the cell with the (b) Co-N-C/SeS_2, (c) SP-Co/SeS_2, and (d) SP/SeS_2.

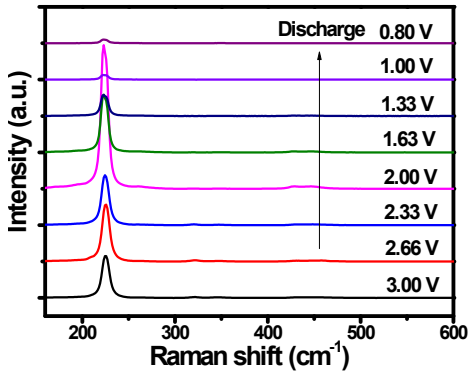


Figure S11. Selected original Raman spectra, as corresponding to Figure 4a.

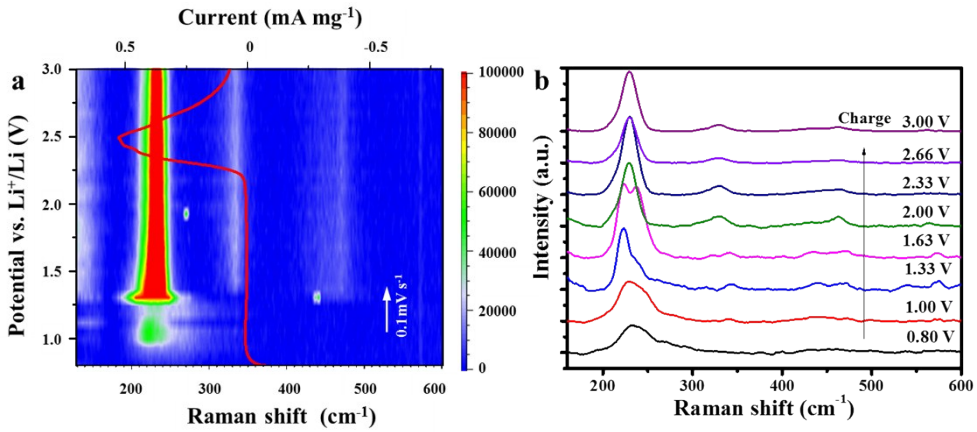


Figure S12. (a) CV curves and contour plot of Raman spectra of the Co-N-C/SeS_2 electrode recorded in the initial anodic scan. (b) Selected original Raman spectra, as corresponding to a.

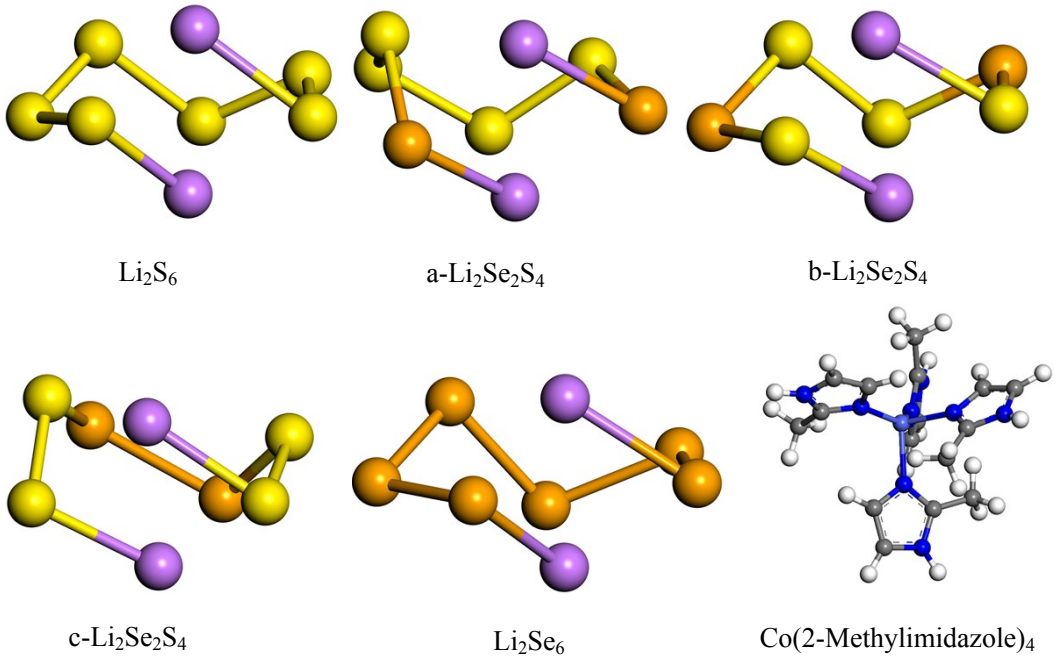


Figure S13. DFT optimized adsorption structures of Li_2S_6, a-$Li_2Se_2S_4$, b-$Li_2Se_2S_4$, c-$Li_2Se_2S_4$, Li_2Se_6 and Co(2-Methylimidazole)$_4$. Co(2-Methylimidazole)$_4$ is a basic chemical unit is used to represent ZIF-67. Pink denotes Li, orange denotes Se and yellow denotes S.

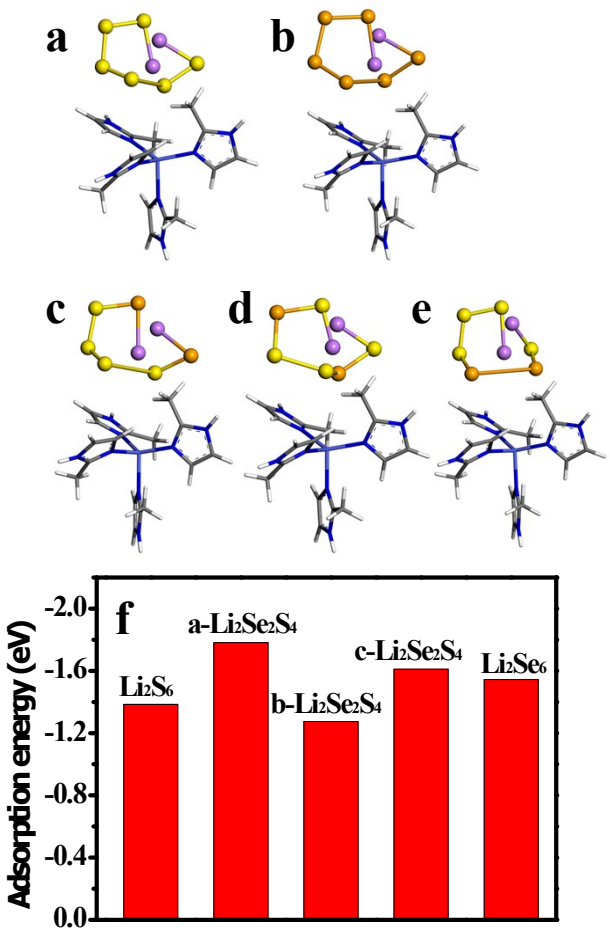


Figure S14. Calculated adsorption energy of (a) Li_2S_6, (b) Li_2Se_6, (c) a-$Li_2Se_2S_4$, (d) b-$Li_2Se_2S_4$, and (e) c-$Li_2Se_2S_4$ on Co-N-C surface. (f) Calculated adsorption energy between Co-N-C and Li_2S_6, $Li_2Se_2S_4$ and Li_2Se_6, respectively.

Table S1. BET surface area, pore size, and pore volume of the Co-N-C and Co-N-C/SeS_2.

	pore size (nm)	pore volume ($cm^3\ g^{-1}$)	surface area ($m^2\ g^{-1}$)
Co-N-C	1.9	0.72	296
Co-N-C/SeS_2	2.7	0.09	70.7