

Supporting information

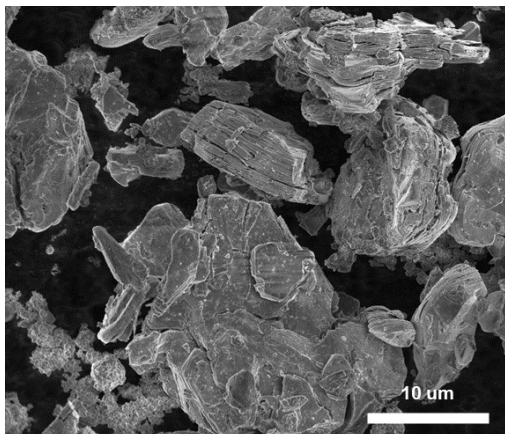


Figure S1. SEM image of the CrSSe powder.

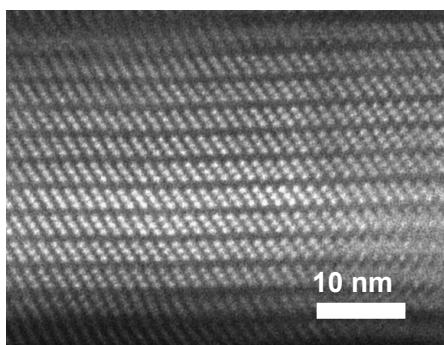


Figure S2. STEM image of CrSSe.

Table S1. Results of Rietveld refinement of CrSSe.

Space group: P -3 m 1 Rwp=1.79% Rp=1.37% $\chi^2=2.075$						
a=b=3.282867(387) Å			c=5.779645(851) Å		$\alpha=\beta=90^\circ$ $\gamma=120^\circ$	
V=53.943(17) Å						
Atom	Wyckoff position	x/a	y/b	z/c	Occupancy	100*Uiso
Cr1	1a	0.000000	0.000000	0.036395	1.0	5,868
S1	1b	0.333333	0.666667	0.207528	0.5	20.615
S2	1c	0.666667	0.333333	0.764392	0.5	-0.081
Se1	1b	0.333333	0.667667	0.219123	0.5	6.700
Se2	1c	0.666667	0.333333	0.765029	0.5	-0.256

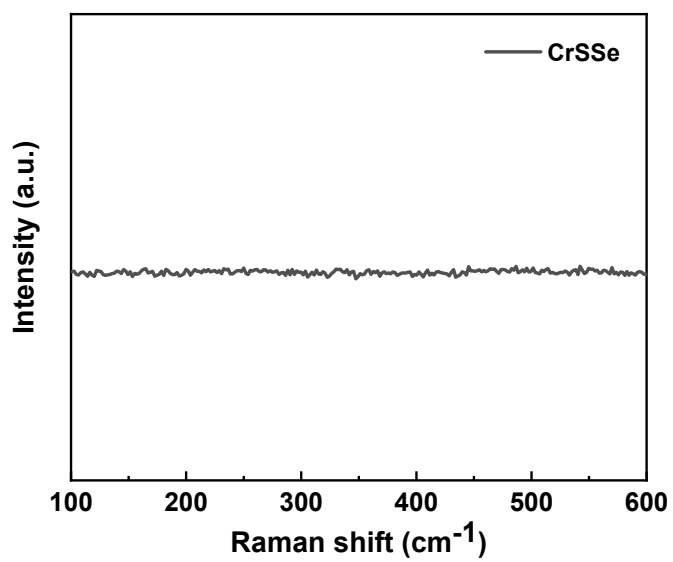


Figure S3. Raman spectrum of CrSSe.

Figure S4. The linear relationship between peak current and the square root of scan rate.

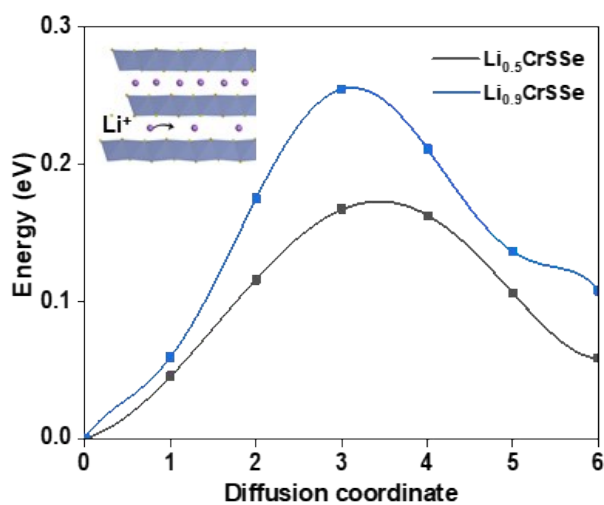


Figure S5. Calculated Li⁺ diffusion barrier in Li_xCrSSe (when x=0.5 and 0.9).

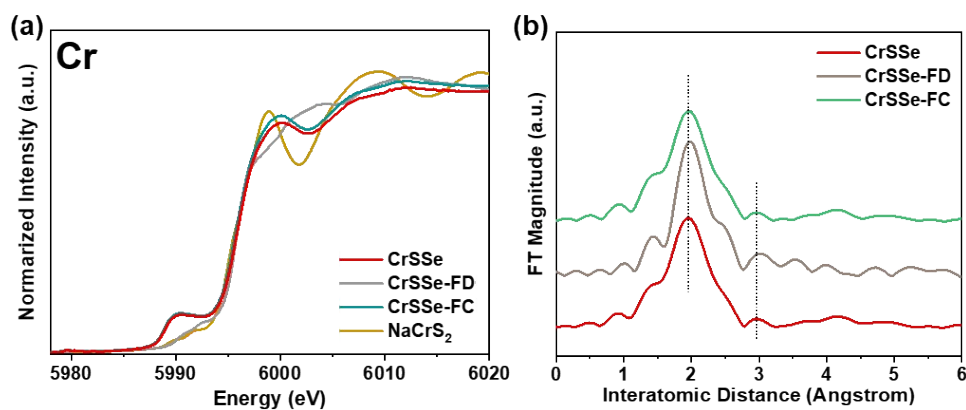


Figure S6. (a) Cr K-edge XANES for NaCrS₂ and various states of CrSSe electrodes; (b) corresponding FT-EXAFS spectrum for various states of CrSSe electrodes.

Table S2. Bond lengths of Cr-Cr and Cr-S/Se in Cr K-edge EXAFS spectrum of various states of CrSSe electrodes. (These values are ~0.4 Å shorter than the real ones, for they have not been phase corrected.)

	CrSSe	CrSSe-FD	CrSSe-FC

Cr-S/Se	1.96	1.97	1.96
Cr-Cr	2.97	3.01	2.97

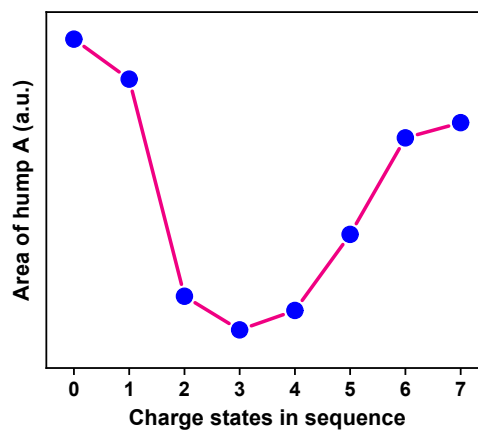


Figure S7. The variation of hump A area along with the charge states in sequence according to the S K-edge XAS spectrum of CrSSe electrode; linear fitting curves of two intermediated states.

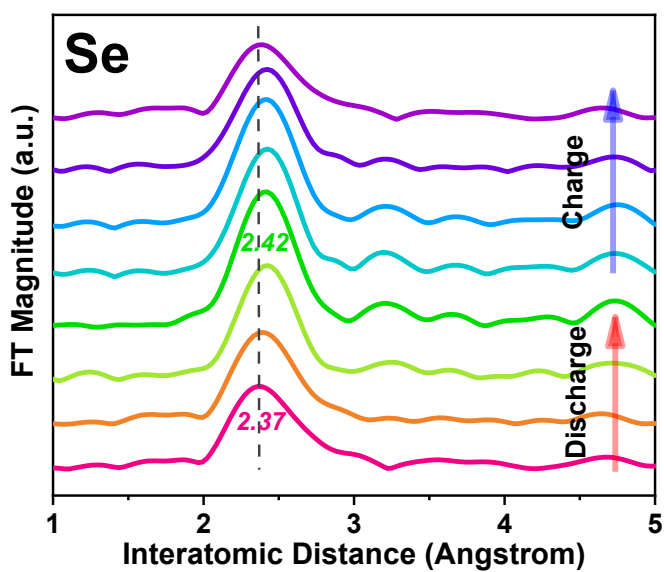


Figure S8. Se K-edge FT-EXAFS spectrum of CrSSe electrode.

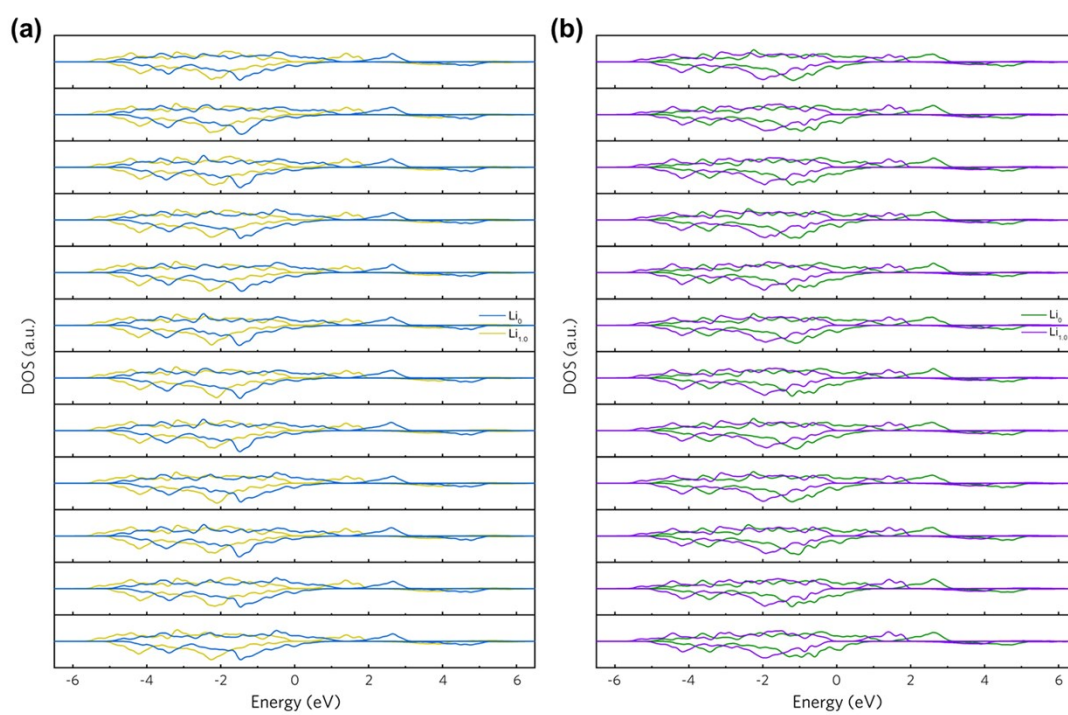


Figure S9. Partial density of states (PDOSs) of (a) S-3p and (b) Se-4p for CrSSe and LiCrSSe.

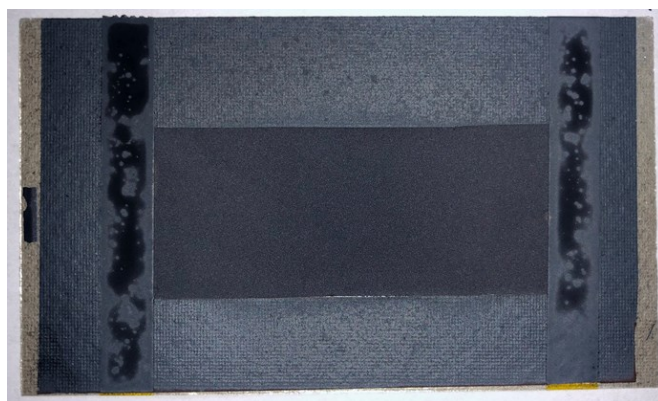


Figure S10. Photograph of CrSSe electrode coated with Fix.Li₃N.

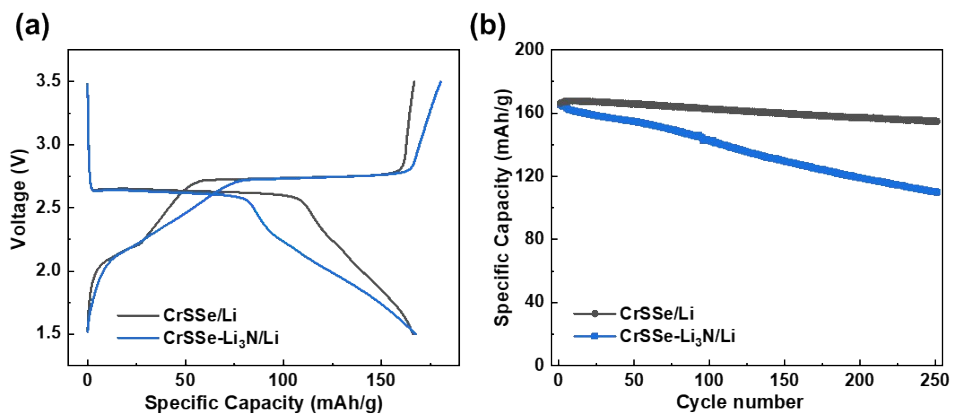


Figure S11. (a) Charge-discharge curves and (b) cycling performance of CrSSe-Li₃N/Li half-cell.

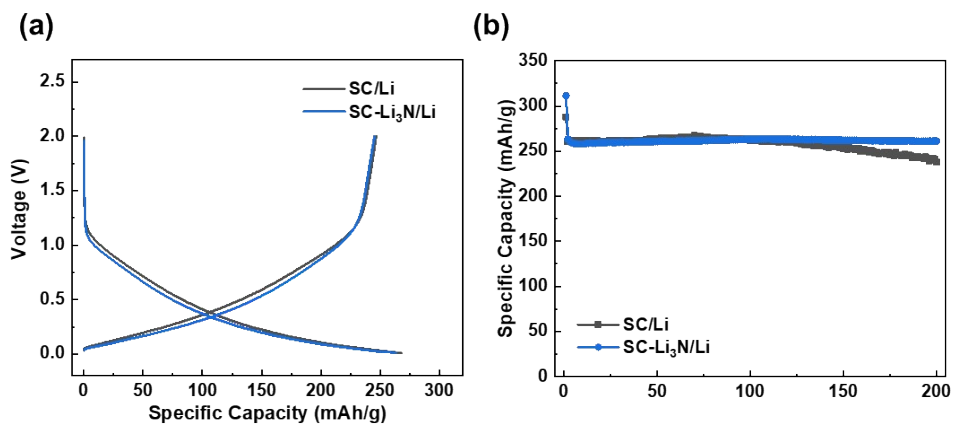


Figure S12. (a) Charge-discharge curves and (b) cycling performance of SC-Li₃N/Li half-cell.