

ESI

Enhanced electrochemical performance of Li-Co-BTC ternary metal-organic frameworks as cathode materials for lithium-ion batteries

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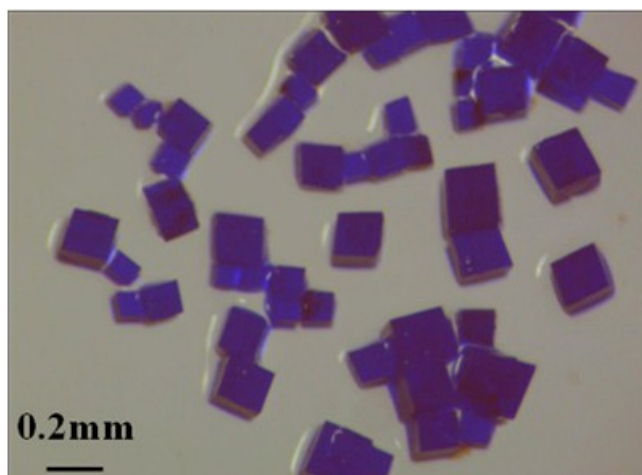
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Table S1. Bond lengths [Å] and angles [deg] for SNNU-74.

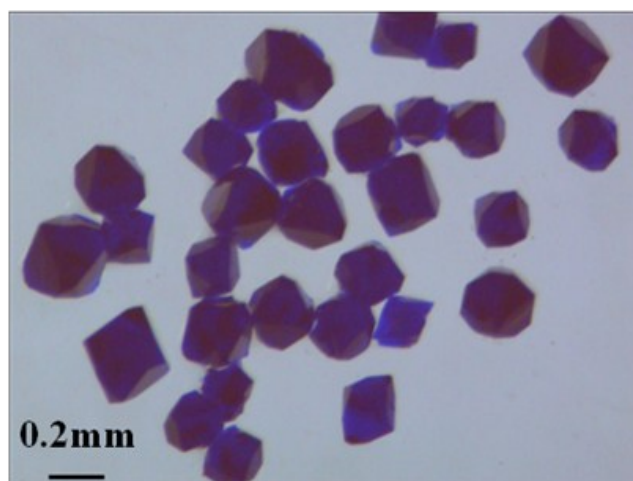
Co(1)-O(5)	1.9323(19)	Li(1)-O(1a)	1.950(5)
Co(1)-O(2a)	1.9335(18)	Li(1)-O(7)	2.078(5)
Co(1)-O(4b)	1.9513(17)	Li(2)-O(8)	1.904(6)
Co(1)-O(7)	1.9832(17)	Li(2)-O(6)	1.914(5)
Li(1)-O(11)	1.906(5)	Li(2)-O(9)	1.973(6)
Li(1)-O(3b)	1.920(5)	Li(2)-O(10)	1.885(6)
O(11)-Li(1)-O(3b)	113.1(2)	O(11)-Li(1)-O(7)	112.2(2)
O(11)-Li(1)-O(1a)	119.6(3)	O(3b)-Li(1)-O(7)	99.5(2)
O(3b)-Li(1)-O(1a)	108.0(2)	O(1a)-Li(1)-O(7)	102.1(2)
O(5)-Co(1)-O(2a)	110.81(9)	O(10)-Li(2)-O(8)	114.8(3)
O(5)-Co(1)-O(4b)	96.14(8)	O(10)-Li(2)-O(6)	115.0(3)
O(2a)-Co(1)-O(4b)	108.90(9)	O(8)-Li(2)-O(6)	113.0(3)
O(5)-Co(1)-O(7)	122.49(8)	O(10)-Li(2)-O(9)	109.4(3)
O(2a)-Co(1)-O(7)	113.39(9)	O(8)-Li(2)-O(9)	103.1(3)
O(4b)-Co(1)-O(7)	102.36(8)	O(6)-Li(2)-O(9)	99.5(3)

Symmetry codes:

a): $-y+1/3, x-y-1/3, z-1/3$; b): $-x+2/3, -y+1/3, -z+1/3$.

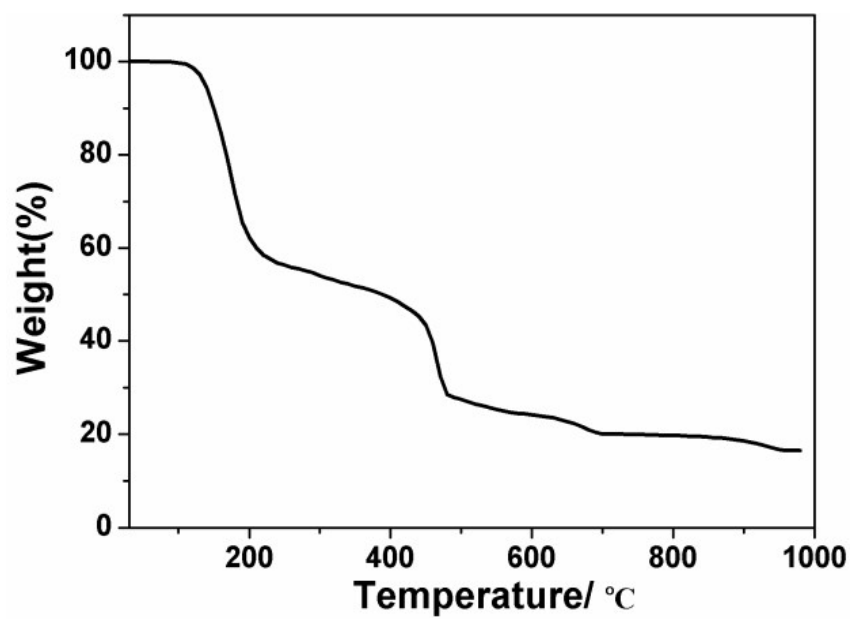


(a)

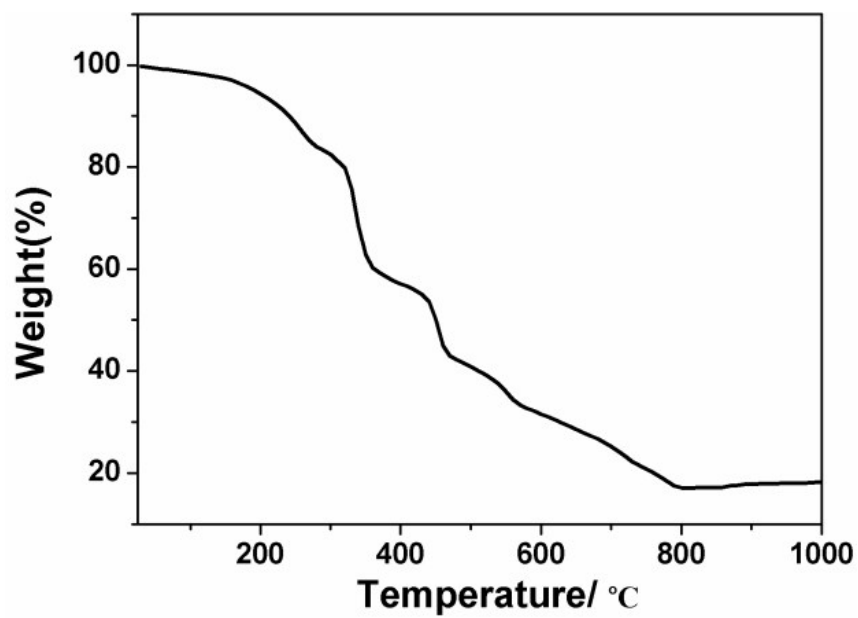


(b)

Figure S1. The photos of SNNU-73 (a) and -74 (b).



(a)



(b)

Figure S2. TGA curves of SNU-73 (a) and -74 (b).

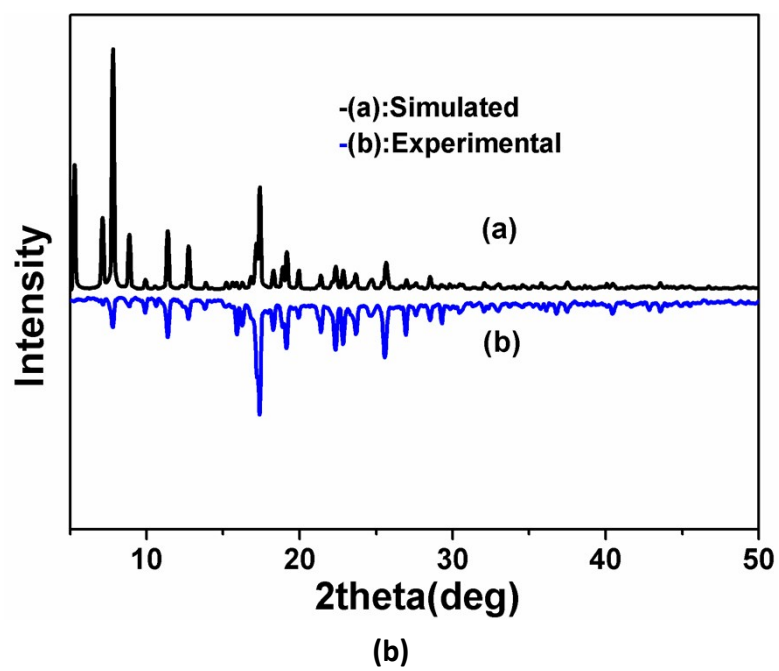
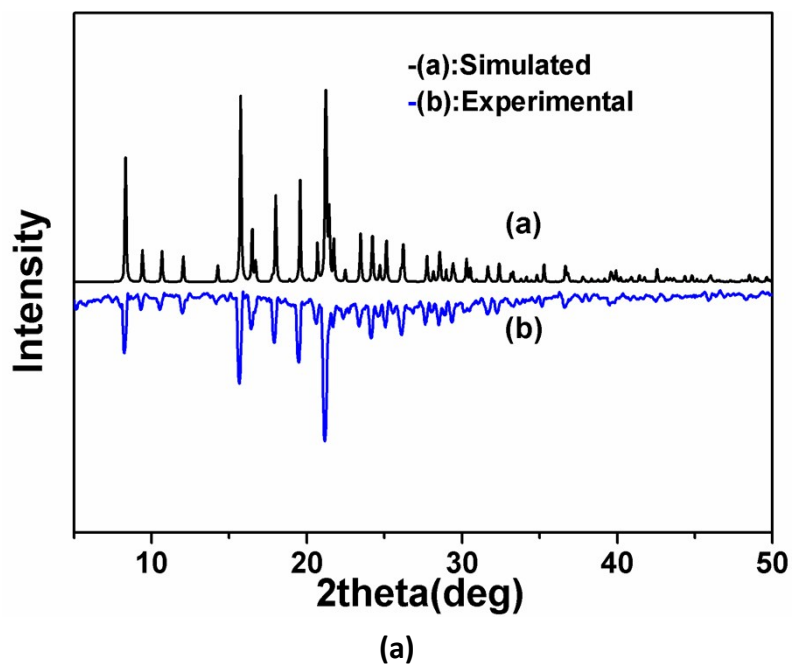
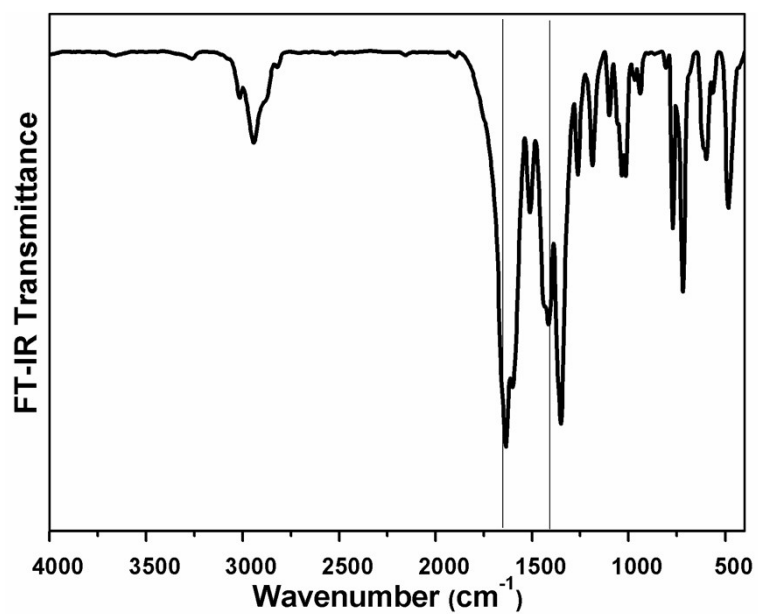
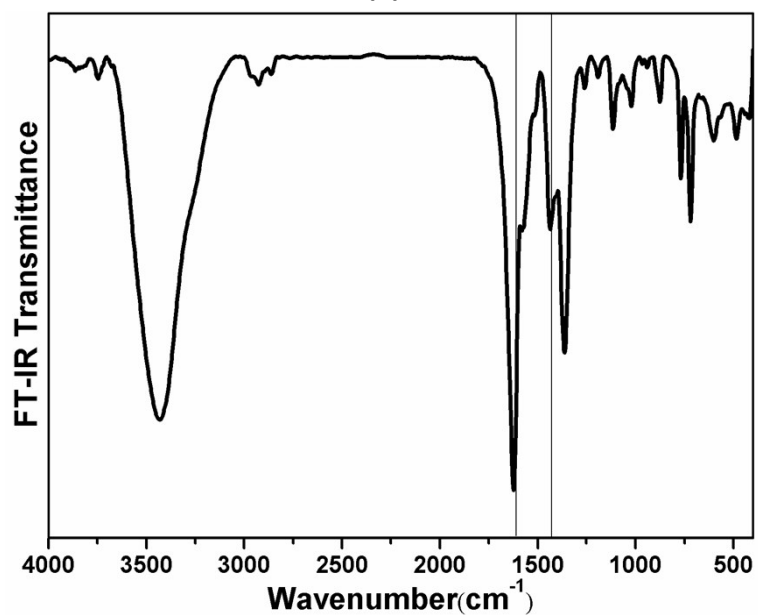


Figure S3. The PXRD pattern of SNNU-73 (a) and -74 (b).

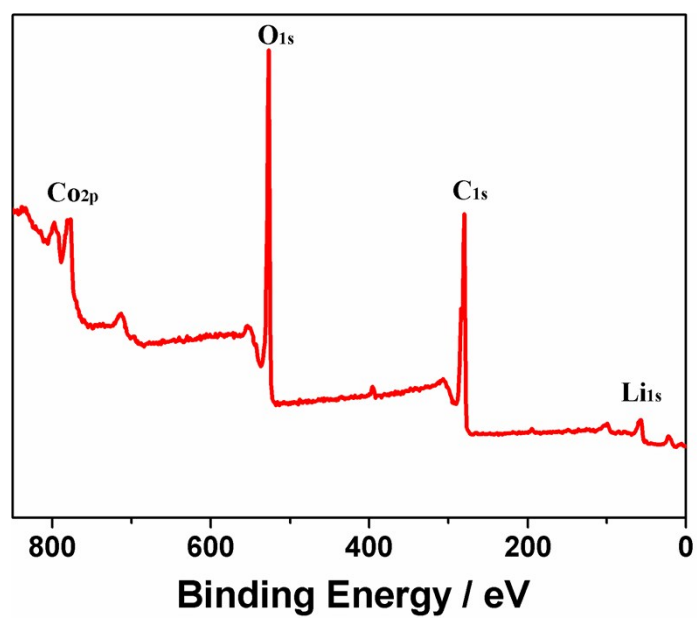


(a)

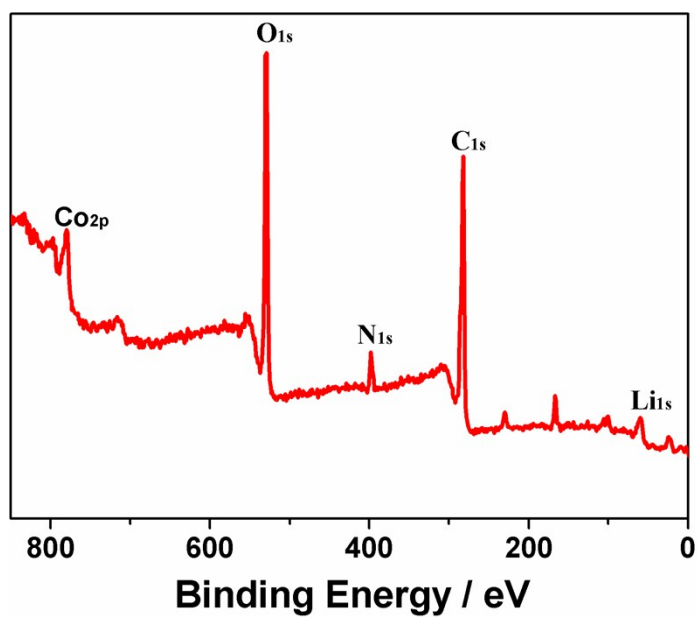


(b)

Figure S4. FT-IR spectra of SNU-73 (a) and -74 (b). The absorption bands in the range of 1340-1620 cm⁻¹ are assigned to the carboxylate groups.



(a)



(b)

Figure S5. The XPS pattern of SNU-73 (a) and -74 (b).

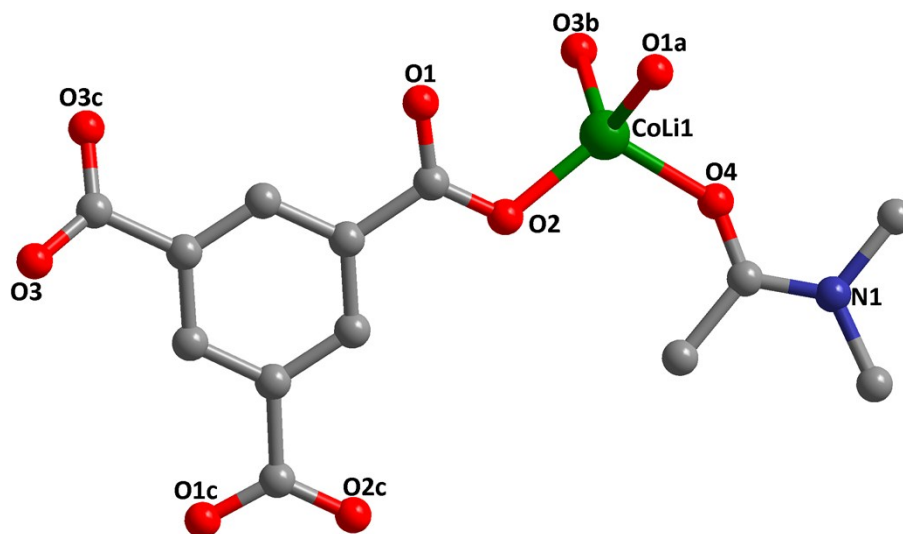


Figure S6. The coordination environments of mixed Co/Li sites in SNNU-73.

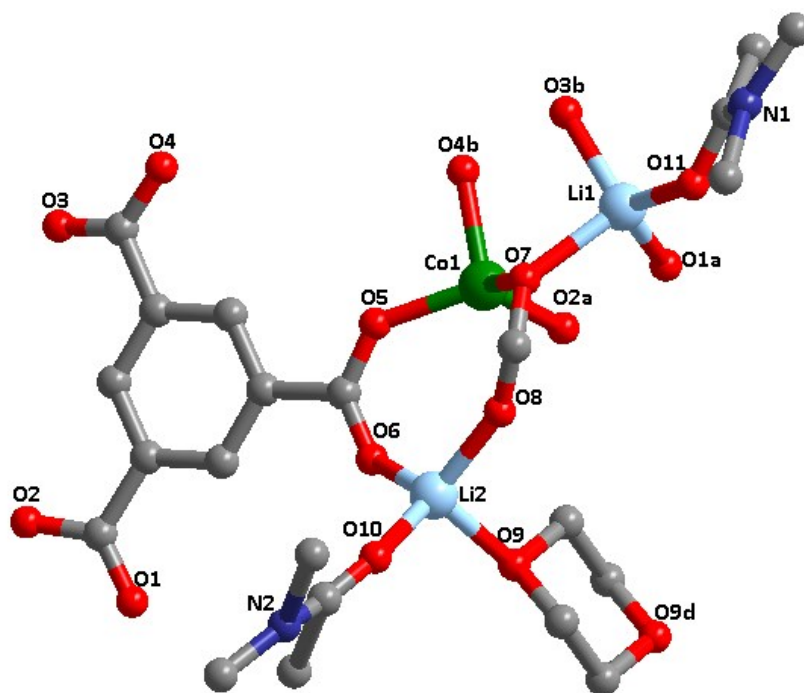


Figure S7. The coordination environments of discrete Co(II) and Li(I) sites in SNNU-74.

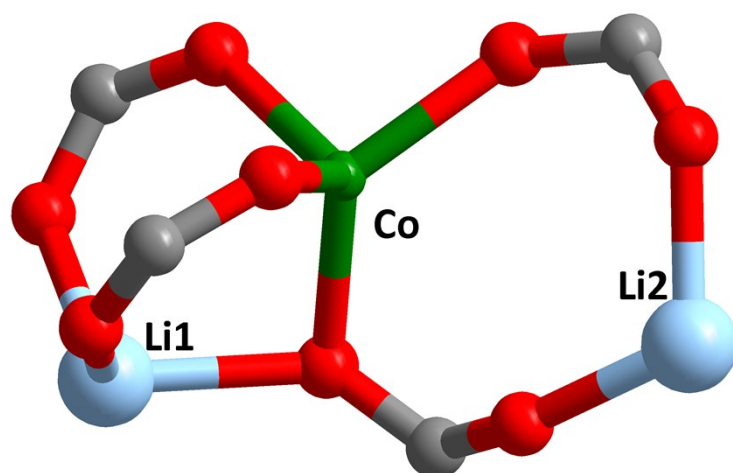


Figure S8. The $[\text{CoLi}_2(\text{COO})_4]$ cluster in SNU-74.

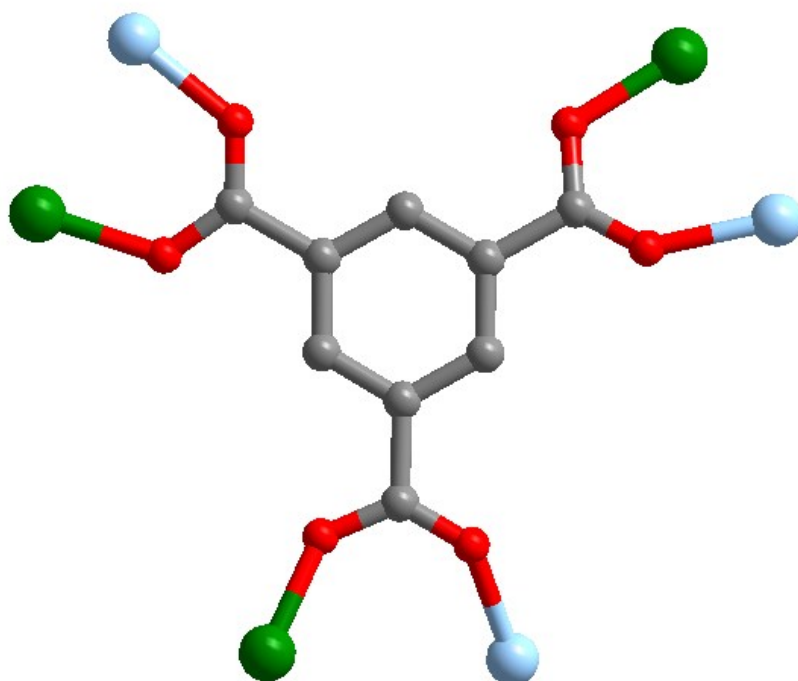


Figure S9. The linkage of H_3BTC ligands in SNU-74.

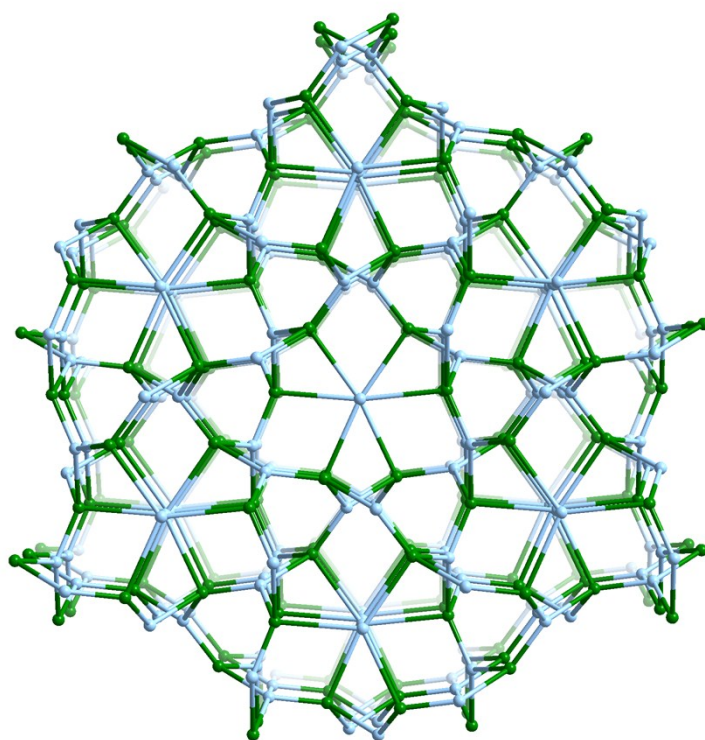


Figure S10. The 3,3,5-connected topological net of SNU-74 viewed along the *c* axis.

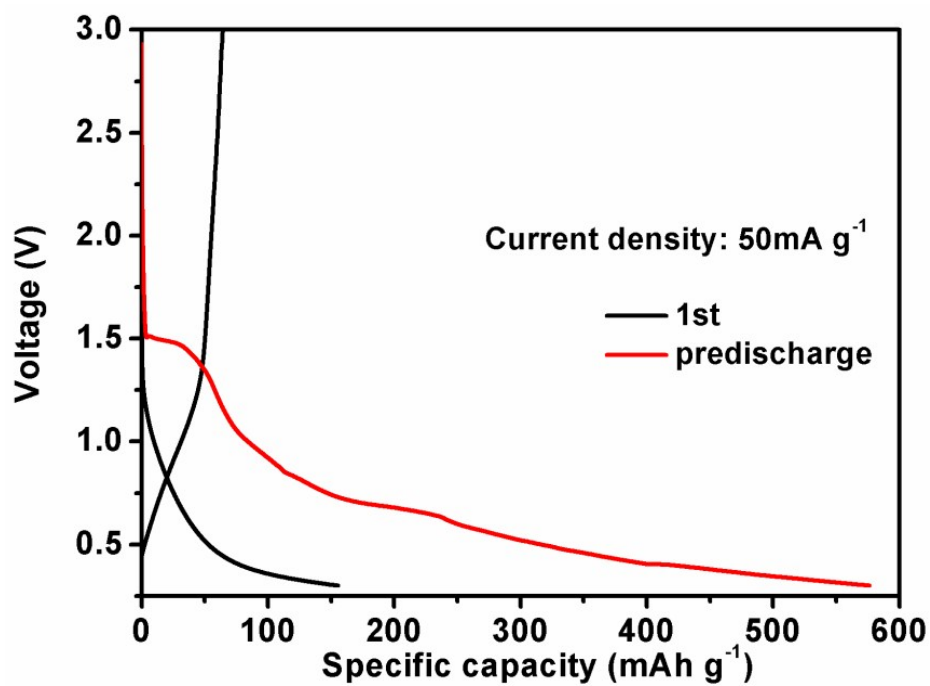


Figure S11. The predischarge curve of SNNU-73 electrode.

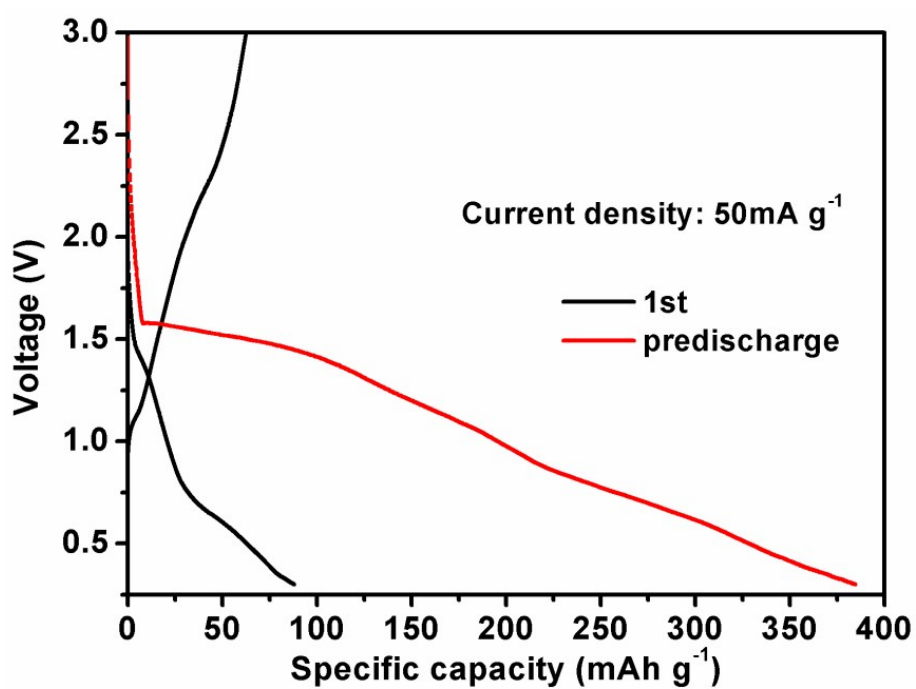


Figure S12. The predischarge curve of SNNU-74 electrode.