Electronic Supplementary Information(ESI) for

Li_3MRuO_5 (M = Co, Ni), New Lithium-Rich Layered Oxides Related to $LiCoO_2$: Promising Electrochemical Performance for Possible Application as Cathode Materials in Lithium Ion Batteries

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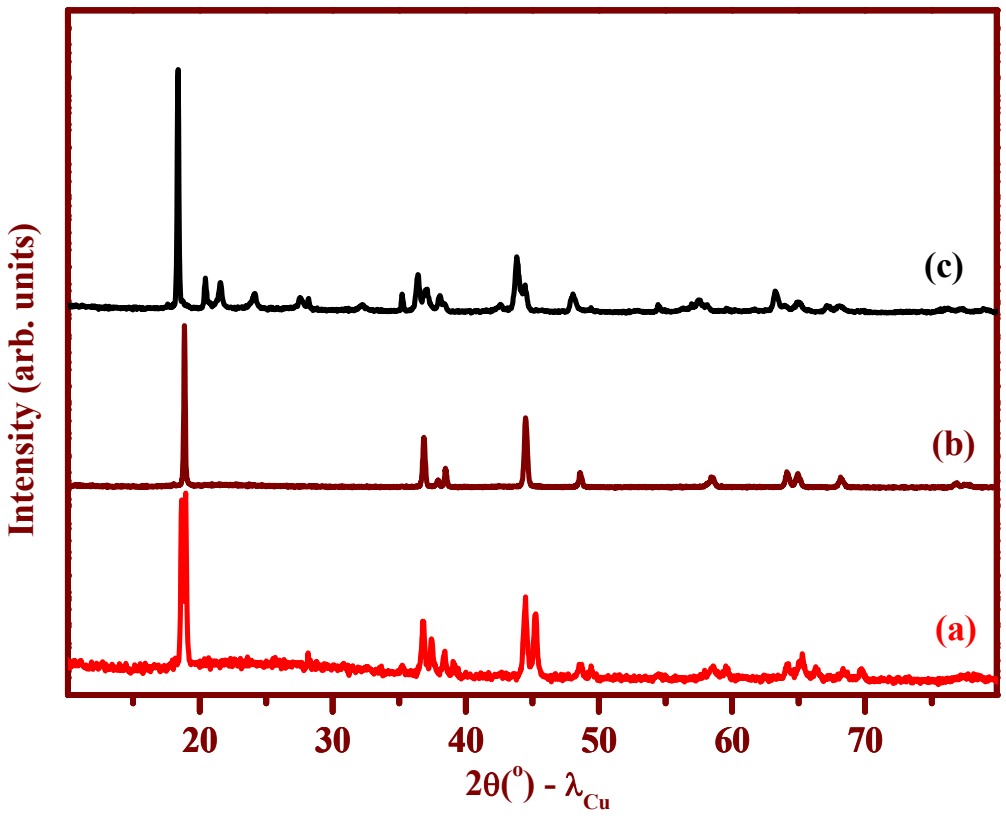

Fig. S1. PXRD patterns of $Li(Li_xCo_{1-3x}Ru_{2x})O_2$: (a) x = 0.1; (b) x = 0.2; (c) x = 0.3.

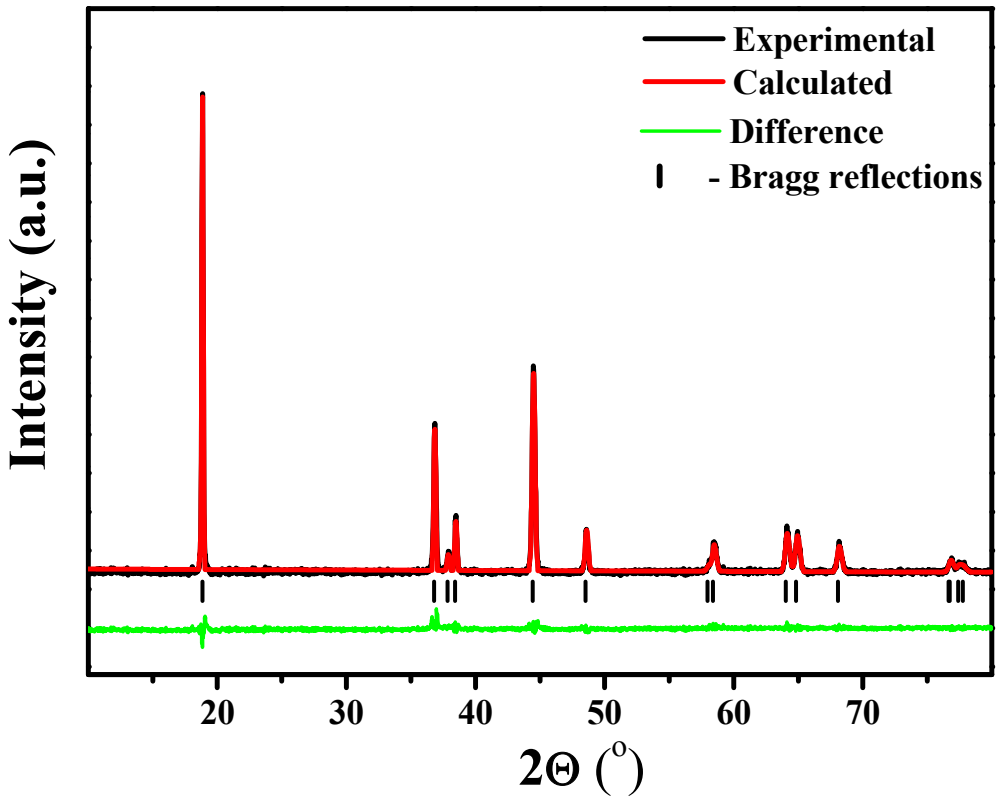

Fig. S2. Rietveld refinement of the structure of Li_3CoRuO_5 from PXRD data.

Table S1. Atomic coordinates and isotropic displacement parameters (U_{iso}) for Li_3CoRuO_5.

Atom	site	x	y	z	U_{iso}(Å^2)	Occupancy
Li	3(a)	0	0	0	0.047(8)	0.977(1)
Co	3(a)	0	0	0	0.036(9)	0.023(1)
Ru	3(a)	0	0	0	0.036(9)	0.000(1)
Li	3(b)	0	0	0.5	0.047(8)	0.223(1)
Co	3(b)	0	0	0.5	0.010(1)	0.377(1)
Ru	3(b)	0	0	0.5	0.010(1)	0.400(1)
O	6(c)	0	0	0.245(1)	0.008(2)	1.000

Space group R-3m, a = 2.888(1), c = 14.387(1) Å

Reliability Factors: R_p = 5.90, R_{wp} = 8.87, R_F^2 = 4.84, χ^2 = 1.33

Bond Lengths (Å): Li(3a)−O = 2.094(1)×6 ; Li/Co/Ru(3b)−O = 2.015(1) ×6

Bond Angels (°): O(1)−Li/Co/Ru(3a)−O(2) = 87.18(1); O(1)−Li/Co/Ru(3a)−O(3) = 92.82(1); O(1)−Li/Co/Ru(3b)−O(2) = 91.58(1); O(1)−Li/Co/Ru(3b)−O(3) = 88.42(1)

Bond valence sums: Li (3a) = 1.10; Co(3a) = 1.72;Li (3b) = 1.36; Co (3b) = 2.16; Ru (3b) = 3.68