

Layered transition metal oxides have been recognised as appropriate cathodes for lithium-ion batteries because to their favourable voltage window, resulting in improved specific capacity and energy density. This work introduces a collection of ternary layered transition metal oxides:  $\text{LiNi}_{0.80}\text{Cu}_{0.10}\text{Nb}_{0.10}\text{O}_2$ ,  $\text{LiNi}_{0.80}\text{Y}_{0.10}\text{Nb}_{0.10}\text{O}_2$  and  $\text{LiNi}_{0.80}\text{Zn}_{0.10}\text{Nb}_{0.10}\text{O}_2$ , synthesised by the hydrothermal process. XRD data demonstrate that all compounds display a hexagonal structure characterised by the R-3m space group. The pattern can be seen for the prepared specimens after their heating at 750 °C for 20 hours in an air furnace. The synthesised materials displayed single-phase diffraction patterns with precisely sharp peaks. This signifies the elevated crystallinity of the powder cathode materials. Notably, impurity peaks were absent in the manufactured samples. SEM micrographs demonstrated the formation of sharply separated particles with various shapes. The crystal structure was produced using Wien2k software, with the lattice constants established using experimental data of the prepared sample. The computed spin-polarized electronic band structures and density of states (DOS) for all three substances demonstrated metallic characteristics. The ferromagnetic properties of the substitutional material are verified by the negative(-ve) values of the exchange constants ( $N_{\sigma\alpha}$  and  $N_{\sigma\beta}$ ). Theoretical estimates of average intercalation voltages (AIV) were obtained from the total-energies( $E_{\text{tot}}$ ) of the optimised compounds and their di-lithiated phases. An electrochemical examination revealed that the theoretical discharge capacities and AIV for the ternary layered transition metal oxides  $\text{LiNi}_{0.80}\text{X}_{0.10}\text{Nb}_{0.10}\text{O}_2$  (X=Cu, Zn, Y) were 1547 , 1543, 1489 mAhg<sup>-1</sup> and 4.4 , 5.4 , 5.5 V, respectively. Experimental and computational investigations suggest the analysed ternary layered transition metal oxides are suitable cathode materials for coin cell manufacturing.