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Determine the Mn-rich phases of transition metal carbonate precursors using Universal Cluster Expansion code

Of all the different types of batteries available and currently developed, lithium-ion batteries (LIBs) have gained a significant segmentation in the market and are the most promising and the fastest growing battery technology. However, the performance of any Li-ion battery greatly depends on the physical and chemical properties of the cathode material, which serves as a host for Li ions. As such, three classes of metal oxide cathodes such as olivine, spinel and layered have been discovered. From the transition metal oxides discovered, this study focuses on the layered composites as they have recently attracted a lot of interest, as the alternative high energy density cathode due to their low cost and less toxicity as compared to other commercialized cathodes for lithium ion batteries. This study reports first-principles calculations on the structural, thermodynamic, electronic, elastic and dynamic properties of layered transition metal oxide at 0 K. The Universal Cluster expansion code managed to generate the manganese rich phases namely Ni0.3Mn0.5Co0.17CO3, Ni0.17Mn0.67Co0.17CO3, Ni0.13Mn0.75Co0.13CO3, Ni0.17Mn0.84Co0.17CO3 and Ni0.13Mn0.87Co0.13CO3. The results showed the thermodynamic stability as follows: Ni0.13Mn0.87Co0.13CO3 > Ni0.13Mn0.75Co0.13CO3 > Ni0.17Mn0.84Co0.17CO3 > Ni0.17Mn0.67Co0.17CO3 > Ni0.3Mn0.5Co0.17CO3.

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