Understanding electrochemical activity of LiNiO₂ positive electrode material for achieving high capacity

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High energy density of lithium ion battery (LIB) is a critical factor for deploying extended range electric vehicle (EV) and back-ups for solar and wind energy. In LIB, a positive electrode material makes a limitation for achieving high energy density of a cell. In this regard, Ni-rich layered (Ni>50%) materials such as NMC(622) and NMC(811) become increasingly attractive because of their higher capacity than conventional LiCoO₂. Recently, LiNiO₂, the layered material with 100% Ni, receives a lot of attention because of high theoretical capacity, 275mAh/g. However, full-capacity of 100% Ni cathode material was not achieved yet partly because of its structure instability with full extraction of Li.

In this study, we try to understand factors that affect the electrochemical activity of LiNiO₂, especially in 1st cycle to determine whether the theoretical capacity of LiNiO₂ can be achieved or not. Considering that LiNiO₂ undergoes several phase transformations, H1-M-H2-H3, during charge/discharge, we investigate the effects of these structural changes on the electrochemical activity. We found out that the capacity in the charge process is always higher than that in the discharge capacity irrespective of the cut-off voltage, which can control the degree of the phase transition. For example, LiNiO₂ with 4.8V of the cut-off voltage can achieve theoretical capacity in 1st charge process but can’t do in 1st discharge. Even with 4.1V cut-off voltage, which is much lower cut-off voltage than 4.8V, LiNiO₂ in 1st charge process shows much higher capacity than that in 1st discharge process. In this poster, we will discuss about the reason why LiNiO₂ has poor coulombic efficiency with respect to the cut-off voltage.