Understanding electrochemical activity of $LiNiO_2$ 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 $LiCoO_2$. Recently, $LiNiO_2$, 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 $LiNiO_2$, especially in 1^{st} cycle to determine whether the theoretical capacity of $LiNiO_2$ can be achieved or not. Considering that $LiNiO_2$ 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, $LiNiO_2$ with 4.8V of the cut-off voltage can achieve theoretical capacity in 1^{st} charge process but can't do in 1^{st} discharge. Even with 4.1V cut-off voltage, which is much lower cut-off voltage than 4.8V, LiNiO2 in 1^{st} charge process shows much higher capacity than that in 1^{st} discharge process. In this poster, we will discuss about the reason why LiNiO2 has poor coulombic efficiency with respect to the cut-off voltage.