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Effects of Nb-doping on phase evolution and electrochemical performance of Li-rich $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{Li}[\text{Ni}_a\text{Co}_b\text{Mn}_c]$ cathode materials

Li-rich $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{Li}[\text{Ni}_a\text{Co}_b\text{Mn}_c]\text{O}_2$ ($a+b+c=1$) cathode materials are promising candidates for lithium-ion batteries owing to their high practical capacity (250-280 mAh/g). But its practicality is hindered due to the intrinsic voltage fade, large irreversible capacity loss, low rate capability, and structural instability issues. Elemental doping strategies are already shown to be effective in enhancing the rate capability and limiting the voltage decay in these materials. [1] Nb⁵⁺ doping is already tried in Li-rich layered oxide particles are proven to be useful in stabilizing the structure and thereby enhancing the electrochemical performance. [2, 3]. However, an in-depth analysis regarding the effect of Nb⁵⁺ doping in the crystal structure, as well as its mechanistic reactions, of Li-rich layered oxides is lacking. In this work, we combine high-resolution neutron powder diffraction and in-operando synchrotron X-ray powder diffraction to study the detailed crystallographic structure of such materials and the corresponding mechanistic behaviours upon lithiation and delithiation, under the effects of Nb⁵⁺ doping. Nb⁵⁺ ions doped into the transition metal ions sites will not only expand the layered structure, improving Li-ion diffusion and hence the rate capability,[2], but also, more importantly, Nb⁵⁺ ions may tune the lattice oxygen activities, accompanied phase transition and structural degradations which are believed to be the root cause of discharge voltage fading in Li-rich layered oxides.

References

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