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Revealing the origin of additional voltage steps of over-lithiated high voltage spinel

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High voltage spinel LiNi0.5Mn1.5O4 is considered as one of the most promising cathode material for next generation lithium ion batteries. The material is expected to be significantly cheaper and more safe than state of the art layered oxides, while providing high specific energy of 690 Wh/kg. Yet this material possesses another highly interesting feature which is the possibility of over lithiation up to x=2.5 in LixNi0.5Mn1.5O4. Utilizing the full compositional range 0<x<2.5, nickel manganese spinel theoretically provides up to 1190 Wh/kg. However, cycling the material to full extend leads to pronounced capacity fading. The reason for this aging is not yet understood and so are the additional voltage step at 2.1 observed during lithiation and the linear voltage slope from 2.0 to 1.5 V, and the additional voltage step at 3.8 V observed during de-lithiation. Only by applying several complementary characterisation methods as operando XRD, neutron diffraction and potentiostatic entropymetry, we were able to attribute the voltage steps to a tetragonal phase of the spinel with lithium ions on octahedral and tetrahedral sites and a metastable cubic phase with lithium ions also located on both octahedral and tetrahedral sites. Therefore this work provides the basis for further material design.

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