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Structure evolution in LNMO, a novel cathode material for Li-ion batteries

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High voltage spinel LNMO is one of the most promising next-generation cobalt-free cathode materials for Li-ion batteries. Besides the typical compositional range of LixNi0.5Mn1.5O4 (0 < x < 1) in the voltage window 4.90 to 3.00 V, additional Li can be introduced into the structure in an extended voltage range to 1.50 V. Theoretically, this leads to significant increase of the specific energy from 690 to 1190 Wh/kg. However, utilization of the extended potential window leads to rapid capacity fading, voltage polarization that lack a comprehensive explanation.

In this work, we conducted operando XRD and neutron diffraction on the ordered stoichiometric spinel LixNi0.5Mn1.5O4 within 0 < x < 2.5 in order to understand the dynamic structure evolution and correlate it with the voltage profile [1]. We were able to provide a conclusive explanation for the additional voltage step at 2.10 V, the sloping voltage profile below 1.80 V, and the additional voltage step at ~3.80 V.

[1] Nicola M. Jobst, Neelima Paul, Premysl Beran, Marilena Mancini, Ralph Gilles,Margret Wohlfahrt-Mehrens, and Peter Axmann, J. Am. Chem. Soc. 2023, 145, 4450–4461

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