

# Experimental report

01/03/2024

**Proposal:** EASY-1084

**Council:** 10/2022

**Title:** Influence of transition metal order and stoichiometry on physico-chemical properties of high voltage LNMO cathode spinel material

**Research area:** Materials

**This proposal is a new proposal**

**Main proposer:** Marcus FEHSE

**Experimental team:**

**Local contacts:** Emmanuelle SUARD

**Samples:**  $\text{LiNi}_{0,5}\text{-zMn}_{1,5}\text{+zO}_4$

Instrument	Requested days	Allocated days	From	To
D2B	5	5	29/03/2023	30/03/2023

**Abstract:**

The main objective for these measurements is to determine the degree of TM order and the Ni/ Mn ratio within two different spinel based  $\text{LiNi}_{0,5}\text{-zMn}_{1,5}\text{+zO}_4$  high voltage cathode materials. It has been shown that both the stoichiometry as well as TM degree have strong influence on the electrochemical performance as a lithium ion cathode active material. Determining crystal structure and stoichiometric properties is therefore required to link them to the electrochemical properties to elucidate the physico-chemical dependencies.

# Proposal EASY-1084 – Experimental report

Main proposer: Marcus Fehse

Local contact: Emmanuelle Suard

## Influence of transition metal order and stoichiometry on physico-chemical properties of high voltage LNMO cathode spinel material

$\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$  (LNMO) spinel is the most promising candidate as cathode material for 3b-generation Lithium ion batteries (LIB) that can meet the high energy density demands set by the automotive sector, while at the same time avoiding environmentally and ethically burdened cobalt. Its high energy density stems primarily from the elevated operating voltage of the  $\text{Ni}^{2+/4+}$  redox couples at 4.7V vs.  $\text{Li}^+/\text{Li}$ .

The main objective for these measurements is to determine the degree of TM order and the Ni/ Mn ratio within two different spinel based  $\text{LiNi}_{0.5-z}\text{Mn}_{1.5+z}\text{O}_4$  high voltage cathode materials. It has been shown that both the stoichiometry as well as TM degree have strong influence on electrochemical performance as a lithium ion cathode active material. Determining crystal structure and stoichiometric properties is therefore required to link them to the electrochemical properties to elucidate the physico-chemical dependencies. The patterns of two LNMO with different degree of TM ratio (Ni/Mn) and TM ordering were successfully acquired at D2b using 1.594Å wavelength. The Rietveld refinement proved suitable to quantify these differences, revealing Ni deficiency and elevated degree of TM ordering for the LNMO-48. These findings have been used in our recent publication references and acknowledging this proposal and previous related proposals, see Enkubahri et al. <https://pubs.rsc.org/en/content/articlehtml/2023/ta/d3ta04649d>

