



Contribution ID: 21

Type: Poster

## Antisite Li\Ni disorder in the NCA-type battery cathode

*Friday, December 9, 2022 3:30 PM (1h 30m)*

The electrochemical efficiency of Li-ion batteries is largely determined by the diffusivity of Li ions and the transport of electrons between electrode materials in the cell. In nickel-containing cathode materials the mixed Li\Ni occupations often occurs, leading to structural disorder, blocking of the 2D diffusion pathways of  $\text{Li}^+$  by  $\text{Ni}^{2+}$ , as well as the reduction of the capacity and structure stability. Mixed transition metal batteries like  $\text{Li}(\text{Ni},\text{Co},\text{Al})\text{O}_2$  and high nickel content  $\text{Li}(\text{Ni},\text{Mn},\text{Co})\text{O}_2$  are considered to be promising cathode materials showing better cycling stabilities, lower toxicity, lower costs etc. and are therefore of particular interest from the viewpoint of Li\Ni disorder [1, 2]. In literature, the studies and understanding of factors causing cation mixing is still controversial and are poorly presented. In the current contribution structural parameters of selected nickel-containing cathodes, obtained by neutron powder diffraction with the instrument SPODI at FRM II will be discussed together with their electrochemical characteristics.

[1] J. Zheng, Y. Ye, T. Liu, Y. Xiao, C. Wang, F. Wang and F. Pan, Ni/Li Disordering in Layered Transition Metal Oxides: Electrochemical Impact, Origin, and Control, *Acc. Chem. Res.* 52, 2201-2209 (2019).

[2] O. Dolotko, A. Senyshyn, M. J. Mühlbauer, K. Nikolowski and H. Ehrenberg, Understanding structural changes in NMC Li-ion cells by in situ neutron diffraction, *Journal of Power Sources* 225, 197-203 (2014).

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**Session Classification:** Poster Session

**Track Classification:** Structure Research