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On the X-ray photoelectron spectroscopy analysis of LiNixMnyCozO2 (NMC) battery electrodes

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Positive electrodes based on lithium-nickel-manganese-cobalt oxides (NMC materials) have been quite often characterized with XPS to address ageing mechanisms of NMC materials. Unfortunately, complexity of the multi-element systems containing several transition metals with rich photoelectron and Auger electron spectra turns the XPS analysis of the chemical state and elemental composition into a quite challenging task. In this talk I would like to point attention of the community to two common problems in the interpretation of the XPS spectra of the NMC materials: confusion of Ni2p spectra with Auger electron spectra (FKLL) of fluorine from PVdF binder and from decomposition of the electrolyte, when the XPS spectra are acquired with Al Kα X-ray source; 2) ambiguous fitting of the XPS spectral lines with several Lorentzian-Gaussian shapes leads to doubtful assignments of the oxidation states and questionable conclusions on the ageing mechanisms of the electrode materials. In particular, it pertains to quantification of the Ni3+/Ni2+ ratio in the NMC electrodes. In the talk we detail the common mistakes made when analyzing the Ni3+/Ni2+ ratio and then we present a novel approach to quantify Ni3+/Ni2+ ratio by making use of the satellite structure in the Ni2p spectra, which was generally ignored previously. We have shown that the satellite in the Ni2p spectra of the NMC compounds is mainly originated from the Ni2+ species and we use the intensity ratio between Ni2p3/2 main peak and the satellite to estimate Ni3+/Ni2+ ratio. Applying this approach for commercial NMC333, NMC532, NMC622 and NMC811 powder materials we find good correlation with theoretically predicted values for freshly made materials.

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