SESSION 5: ANODE/CATHODE

LAYERED NA,CO-OXIDES WITH TITANIUM: DESIGN OF OPTIMAL COMPOSITIONS FOR APPLICATION IN SODIUM BATTERIES

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Similar to Li-batteries, Na-batteries require cathode materials with a high energy density, which is a product of the specific capacity and the average working cell potential. To increase the working potential, a presence of Co in the material would be beneficial. Although $NaCoO_2$ as a positive electrode shows a high theoretical capacity, it undergoes numerous phase transformations (electronic and structural) during battery charging and discharging, which impede its long-term operation, especially at high current rates. Moreover, the excessive use of Co is undesirable from environmental and ethical perspectives.
In order to stabilize the crystal structure during Na-removal, a partial substitution of Co by other transition metals, which must not necessarily be redox-active, seems to be a successful strategy. Although the specific capacity may be reduced because of the doping, an increased structural stability would lead to improved kinetics.
In present study, the role of Ti as a structural stabilizer in $Na(Co,Ti)O_2$ materials was elucidated, using a multidisciplinary approach which includes XPS, *operando* XRD and XAS, and magnetization measurements. As an example, we observed only one structural transformation for the $Na_xCo_{0.5}Ti_{0.5}O_2$ composition during desodiation [1], thus confirming the stabilization effect of the Ti-substitution. However, we detected a spin state transition of Cobalt in sodiated and desodiated phases, which results in a significant change of the lattice volume and leads to a big hysteresis between the charge and discharge. In contrast, using of Na-deficient compositions with less Ti substitution provides a close evolution of charge/discharge curves, although a higher number of intermediate phases during battery charge was registered [2,3].

References
[1] S. Maletti at al., *ACS Appl. Mater. Interfaces* 2018, 10, 36108–36119.
[2] N. Sabi at al., *J. Power Sources* 2017, 342, 998-1005.
[3] N. Sabi at al., *ACS Appl. Mater. Interfaces* 2017, 9, 37778-37785.