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STRUCTURAL STUDIES ON TWO-DIMENSIONAL SODIUM OXIDES AS CATHODES FOR NA-ION BATTERIES

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Increased attention to sodium-containing materials during the last years is caused by the rapid development of sodium-ion batteries (NIBs), which are considered as a potential successor for lithium-ion batteries (LIBs). Especially layered sodium oxides with transition metals have gained large interest due to their potential applicability as cathode materials. Similar to $LiCoO_2$ in LIBs, $NaCoO_2$ of the α-$NaFeO_2$ or β-$RbScO_2$ structure type shows an immense potential as a cathode in NIBs. A partial replacement of Co by other redox-active (Ni, Mn, Fe) or inert (Mg, Ti, Sb) metal cations can stabilize the crystal structure during (de)sodiation, and reduce the number of phase transformations. Other class of layered Na-oxides with a $MnO_2 \cdot nH_2O$ birnessite-type structure, also suitable for application as Na-cathodes, is much less investigated, probably due to a difficulty to obtain a water-free materials. Here Mn cations can be partially replaced by other transition metals, while Na-cations can replace H_2O molecules.

Using neutron powder diffraction, we investigated temperature-dependent structural behavior of layered Co-oxides of different structure types in order to optimize the synthesis conditions. Using operando synchrotron diffraction and X-ray absorption spectroscopy, we studied their structural evolution in Na-batteries during charge and discharge. The combination of structural studies facilitated understanding the electrochemical performance of the materials.

Primary author: MIKHAILOVA, Daria (IFW Dresden)

Presenter: MIKHAILOVA, Daria (IFW Dresden)

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