

relation between the anionic redox process and the evolution of the O-O bonding in layered oxides.

Keywords: Li-ion battery, cathode, crystal structure, transmission electron microscopy

MS19-P2 Heterometallic single precursor of oxides for Na-ion battery cathode materials

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After decades of improvements of and investments in the Li-ion battery technology, attention has been shifted toward Na-ion battery, mainly because of sodium's low cost. A lot of different materials are investigated as potential cathode for Na-ion batteries, especially the layered oxides of transition metals, NaT_MO_2 (with $T_M = \text{Ti, V, Cr, Mn, Fe, Co, Ni, \dots}$), which are traditionally synthesized via solid state techniques.

These solid state techniques involve high energy ball-milling of several precursors (usually sodium carbonate and transition metal oxide) followed by calcination at high temperature (800-1000°C) for long reaction times, (8-12 hours) [2]. This long and energy consuming process was required in order to obtain a homogeneous mixing of the precursors. Recently, it was reported that synthesizing heterometallic single precursor can reduce the duration and the calcination temperature due to the pre-organized precursor design [3]. The high temperature phase of lithium cobalt oxide (HT-LiCoO₂) was obtained using heterometallic Li-Co alkoxides/aryloxide complexes as precursors [3] at as low temperatures as 350-450°C instead of 600-900°C required for the solid state synthesis [4].

The crystal structure of Na_xCoO_2 ($x < 1$) has octahedral CoO_2 layers and prismatic coordinated sodium ions (Figure 1)[1]. The content of sodium influences the crystal structure and the lattice parameters of the unit cell. In the end, the amount of sodium in the structure also determines the specific capacity of sodium ion batteries.

We synthesized the Na_xCoO_2 starting from heterometallic complexes of sodium and cobalt. The method of heterometallic complexes is also applied to other transition metals: nickel, iron and manganese. The obtained oxides will be characterized and tested as sodium ion battery cathode materials. We will present our first efforts, results of syntheses and characterizations.

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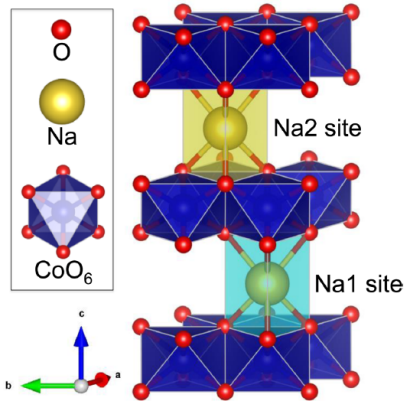


Figure 1. Crystal structure of NaCoO_2 [1]

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MS19-P3 Molecular and Crystal Structures of Aminoalanes and Aminoboranes

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Compounds, bearing $\text{H}^{\delta+}$ and $\text{H}^{\delta-}$ species, are promising candidates for reversible hydrogen storage materials. This strategy has already been discussed, e.g. by Stephan and Erker [1] for Lewis-acid/base adducts, which show a reversible hydrogenation. Lewis-acid/base adducts of nitrogen and aluminium or boron could be economically and environmentally beneficial candidates for hydrogen storage, e.g. in NH_2BH_3 [2, 3]. Within the group 13 elements, Lewis-acid/base adducts with different substituents often form molecular structures build up by dimers or trimers [Figure 1 (a)]. Since, the reactivity of these compounds towards small molecules like H_2 [4] or CO_2 [5] strongly depend on the bond lengths between the corresponding Lewis acid and the base, a knowledge of their molecular structures is crucial for their applications.

Recently, we determined the crystal structure of diethylaminoalane by a combination of powder X-ray diffraction, Raman spectroscopy and DFT calculations [6]. This approach has led to a reliable molecular structure determination of diethylaminoalane in the solid state and to obtain further information about the environment and behavior of the Al-H bonds. This combination of techniques was also applied to characterise a phase transition of dimethylaminoalane [Figure 1 (b)] from a monoclinic to a plastic crystalline phase, where the molecules are found to be strongly disordered and arranged accordingly to the cubic $a15$ phase, often adopted by liquid crystals. The analogous boron compound, dimethylaminoborane, is an example for a substance which can exist as dimer or as a trimer. For dimeric dimethylaminoborane, we were able to determine its monoclinic crystal structure and the second order phase transition to a triclinic phase by single crystal X-ray diffraction and in-situ X-ray powder diffraction. Our measurements confirm the cell parameters from [7], and led to the atomic positions.

References:

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