



Internship or bachelor thesis

Layered oxides with honeycomb ordering as cathode materials for Na-ion batteries

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Layered transition metal oxides Na_xMO_2 (M = transition metal) become popular sodium-insertion materials due to good mobility of Na^+ -ions inside the structure. The honeycomb-ordered phases of general formula $\text{Na}_3\text{M}_2\text{SbO}_6$ (M = Ni, Cr, Cu, Co, etc.) [1] are structurally related to the layered Na_xMO_2 with an $\text{M}^{2+}/\text{Sb}^{5+}$ cationic ordering or a superstructure within each slab, where each SbO_6 octahedron is surrounded by six MO_6 octahedron forming a honeycomb network [2-4]. For $\text{Na}_3\text{Ni}_2\text{SbO}_6$, the theoretical capacity ($199 \text{ mAh}\cdot\text{g}^{-1}$) corresponds to the extraction/insertion of 3 sodium ions per formula unit, which takes place in the high potential range of 3.1-3.8 V vs. Na^+/Na . The total or partial substitution of Sb^{5+} with other M^{5+} cations may result in new high performance battery materials with honeycomb ordering in the transition metal layer. The synthesis of $\text{Na}_3\text{Ni}_2\text{BiO}_6$ has already been reported [5], but the electrochemical characteristics of this compound in sodium-ion cells are still missing. At the same time, it is interesting to explore the possibility of substitution of Sb^{5+} with smaller and lighter V^{5+} in this type of structure. The nominal composition $\text{Na}_3\text{Ni}_2\text{VO}_6$ has not been reported so far.

The aim of this work is to synthesize honeycomb structures of $\text{Na}_3\text{Ni}_2\text{BiO}_6$ and $\text{Na}_3\text{Ni}_2\text{VO}_6$ and to determine their electrochemical performance in sodium-ion cells. The optimization of the synthesis conditions (temperature, annealing protocol, precursors) is required. X-ray powder diffraction and scanning electron microscopy will be used to characterize the crystal structure and morphology of the obtained compounds. The electrochemical potentials and capacities of sodium insertion-extraction will be investigated by galvanostatic cycling and cyclic voltammetry in the electrochemical cell with Na-anode and non-aqueous Na-electrolyte.

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References:

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