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Influence of Structure and Charge Ordering in P2-type Cathode Materials for Sodium-ion Batteries

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With increasing share of energy generation from renewables, intermittent electrical energy storage is gaining significance. Sodium-ion batteries (SIB) are currently developed and commercialized as cost-effective complementary technology to today's Lithium-ion batteries (LIB). For SIBs, P2-type layered oxides are considered amongst the most attractive cathode active materials.
In this work, we have synthesized P2-type NaxMnyNi1-yO2 cathode active materials for SIBs with y = 2/3 and 3/4. The materials are characterized with Neutron and X-ray powder diffraction and advanced electrochemical methods. The material with y = 2/3 exhibits a honeycomb Ni/Mn superstructure and clear potential jumps at distinct sodium contents (x = 2/3, 1/2, 1/3). Based on electrochemical investigations and operando Synchrotron XRD, these voltage jumps are assigned to Na+/vacancy orderings. With increased Mn-content of y = 3/4, the honeycomb Ni/Mn superstructure is disrupted, the potential profile smoothed and the extend of Na+/vacancy orderings reduced. Using first principle calculations (DFT), we demonstrate, that Na+/vacancy ordering is directly related to charge ordering within the transition metal slab. The influence of transition metal charge ordering on Na+/vacancy ordering is discussed and validated against P2-type cathode materials with various transition metal compositions. A general guideline to suppress Na+/vacancy orderings in P2-type cathode materials for SIBs is postulated.

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