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Promising And Anomalous Structural And Electrochemical Properties Of Polyanionic Phosphates In Sodium Ion Batteries

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Abstract

This work presents a recent progress on the polyanionic phosphate family that functions as cathode materials in sodium ion batteries (SIBs). Firstly, this study will cover vanadium-containing frameworks that show very stable voltage curves in different potential regimes with advantageous behaviors such as single flat voltage plateaus and the presence of intermediate phases that are beneficial for cell kinetics. In the second part of our study, some anomalous manganese activation in the SIBs pyrophosphate family that overcomes the chronic Jahn-Teller distortion, in contrast to the Li counterparts will be introduced. By employing density functional theory (DFT) calculations, it is figured out that such anomalous activation is originated from its unique crystal structure where corner-sharing is the main structural change during the phase transformation in the charge-discharge processes. In addition, unique SIBs properties will be compared to the lithium ion batteries (LIBs) analogues even for the same chemical formulae.