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Crystal Structure Study of Manganse Hexacyanoferrate Cathode Material in Organic Na-ion Battery by using XAS and XRD

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Manganese Hexacyanoferrate (MnHCF) as promising electrode material has been wildly used as a cathode in organic Na-ion batteries, and displaying large specific capacity (>130 mAhg-1) and high discharge potential [1]. However, the phase and structure changes of MnHCF associated with the electrochemical reaction, especially the Jahn-Teller (JT) distortion of Mn-sites during the charge process, result in the lower cycling stability. As we reported previously, the X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS) results demonstrate that a non-cooperative JT distortion of Mn sites was observed in Li-ion ansd Na-ion batteries of MnHCF [2, 3].

In order to highlight the influence of framework of MnHCF on the stability of Na-ion battery, we synthesized two MnHCF samples with different vacancy content. The electrochemical result shown that the sample with lower vacancy content (4%) exhibits higher capacity retention (71.1%) after 100 cycles at C/5. Ex-situ XAS and ex-situ XRPD characterization provide insight into the different oxidation states of Metal-sites and the crystal structure change during cycling. We found that the sample with higher vacancy content (11%) exhibits a cooperative JT distortion during cycling, while which is confirmed that not favor to the cycling stability. Instead, the sample with lower vacancy content displayed an irreversible structure changes, and which result in higher cyclability.

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