Comparative study on Li storage mechanism of MoO$_2$/CNTs and MoO$_3$/CNTs composite as anode materials for lithium-ion battery

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Nano-sized Molybdenum oxides (MoO$_x$) are promising electrode materials for efficient lithium storage system because of their high lithium accommodation ability and unique chemical properties.$^{[1]}$ In addition, it was shown that electrical conductivity and electrochemical performance like reversible capacity and rate capability can be improved by introducing carbon materials.$^{[2][3][4]}$ Numerous works on the nanocomposites of MoO$_2$/MoO$_3$ and carbon materials have been previously reported as anode materials for lithium-ion batteries (LIBs). However, most of them were focused on either MoO$_2$ and MoO$_3$ nanocomposite and there has been no systematic and comparative study of lithium storage mechanism of MoO$_2$ and MoO$_3$.

Understanding the lithium storage- and capacity fading-mechanisms is imperative to further improve the electrochemical performance of molybdenum oxide (MoO$_x$) nanocomposites. In this regard, we have systematically investigated lithium storage mechanism of MoO$_x$ by comparing the structural changes occurring in MoO$_2$ and MnO$_3$ nanocomposite electrodes during charging and discharging. In order to explore true structure-property correlations, we have synthesized MoO$_2$/CNTs and MoO$_3$/CNTs nanocomposite materials with very similar morphological features through a simple hydrothermal process followed by heat-treatment. As a result, well-dispersed MoO$_2$ and MoO$_3$ nano-particles partially grown on CNTs were formed. These two nanocomposites showed distinctive differences not only in voltage profile but also in reversibility during electrochemical cycling. By using synchrotron-based x-ray diffraction (XRD) and x-ray absorption spectroscopy (XAS) during cycling, distinctive structural changes between MoO$_2$/CNTs and MoO$_3$/CNTs were systematically compared and investigated to provide insights on how to design molybdenum oxide materials with improved electrochemical performance.

![Figure](image_url)

**Figure.** Discharge and charge curve of MoO$_2$/CNTs and MoO$_3$/CNTs composite

**References:**