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 nano-composites 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.

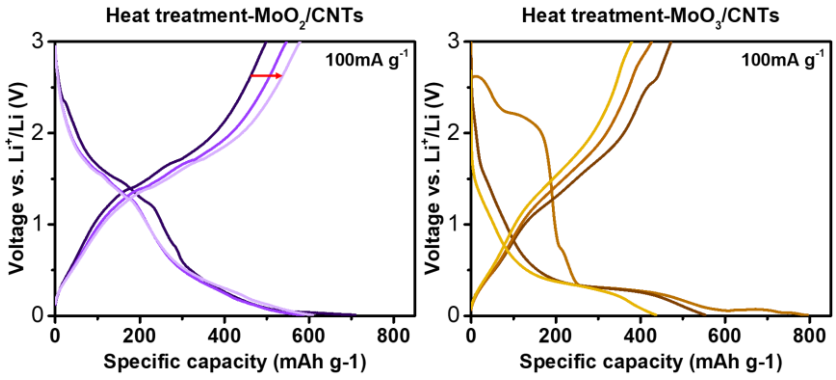

Figure. Discharge and charge curve of MoO_2/CNTs and MoO_3/CNTs composite

References:
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[3] Yongming Sun, Xianluo Hu, ACS NANO, 2011, 5(9), 7100-7107
[4] Feng Ma, Anbao Yuan, ACS Appl. Mater. Interfaces, 2015, 7, 15531−15541