Bulk to Nano : Different reaction pathway of molybdenum disulfide with lithium

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MoS_2 has superior electrochemical properties suit for lithium ion battery, such as high theoretical capacity (670 mAh/g), low volume expansion during cycle (~103%) and the week vdw forces between layers, which offers facile route for Li^+. The lithium storage mechanism of MoS_2 is widely known as an irreversible intercalation reaction in the first cycle and reversible conversion reactions ($MoS_2 + 4Li^+ + 4e^- \leftrightarrow Mo + 2Li_2S$). However, some recent studies contradict above mentioned pathway and suggest different reversible reaction path ($Li_2S \leftrightarrow 2Li^+ + S^{2-}$), similar to the Li-S battery reaction.

In order to clarify the reaction process, we synthesized ordered mesoporous MoS_2 as a model structure to ascertain the complete reaction by obtaining the maximum reversible capacity from this material.

We also utilized synchrotron radiation based characterization techniques to directly observe local and bulk structural changes in the well-synthesized mesoporous MoS_2 during the electrochemical cycling.