Exceptionally high Li storage of nanostructured materials for next generation Li batteries

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Lithium ion batteries (LIBs) are a key-enabling technology for addressing the power and energy demands of electric vehicles and stationary electrical storage for renewable energy as well as mobile electronics.[1] However, the energy density of currently commercialized LIBs is already close to its technological limit.[2] In order to achieve the battery performance that all applications expect, much effort has been made to develop new electrode materials to enhance both the energy density and cycle performance of LIBs.[3] Especially, for improving the performance of anode parts replacing graphite (theoretical capacity of 372 $mAhg^{-1}$), there has been extensive research on developing anode materials such as transition metal oxides, silicon- or tin based metal alloys, and related composite configurations. Since they follow lithium storage mechanisms such as conversion and alloying reactions, which are different from the intercalation reaction in the graphite anode, these newly developed anode materials show higher capacity than the current anode systems. In particular, there had been several reports that some transition metal oxides showed the reversible capacity exceeding their theoretical capacity based on the conversion reaction. This abnormal capacity of transition metal oxides has been explained by various mechanisms based on the interfacial reaction, which approach has the potential to significantly increase the reversible capacity and the rate capability of anode materials by enlarging the interfacial area between the electrode and electrolyte.[4–6] Namely, exploring new reaction mechanism and related novel electrode materials can play a critical role for pushing current battery technology to a next level.

In these studies, we introduce a novel reaction with a new $Co(OH)_2$ material which exhibits an initial charge capacity of 1,112 mAh g^{-1}, about twice its theoretical value based on known conventional conversion reaction, and retains its first cycle capacity after 30 cycles. In order to understand the origin of anomalously high capacity beyond the theoretical value for the conversion reaction as well as detailed lithium storage mechanism, we conducted synchrotron XRD and XAS, AIMD simulation, localized STEM and XPS measurements. These results will provide novel insight for possible lithium storage mechanisms for nanostructured anode materials, and thus enable the innovative design of electrode materials for next generation LIBs. Subsequently, we will also present detailed lithium storage mechanisms for nanostructured anode materials that show anomalously higher capacity than their theoretical limit, at the time of meeting.

References:

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