Applications of in-situ x-ray absorption spectroscopy for next-generation batteries

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The fast pace growth of portable electronics and commercialization of electric vehicles has increased the demand for low cost, high energy density, durable and safer energy storage systems. This has attracted considerable research on developing and improving various types of batteries, including Li/Na ion, Li-S and Li/Na-air batteries. However, changes in the structure and chemistry of these systems with the goal of improving their performance, requires a better understanding of the underlaying process during their operation. Furthermore, continuous monitoring of state of health of batteries during operation is essential for illuminating the degradation mechanisms and formulating methods to address their durability issue.

In our work, we have used ex-situ X-ray absorption spectroscopy as vital tool to study correlation between local electronic and atomic structure of nanostructured cathode and anode electrodes with their performance in various rechargeable batteries [1-5]. To study the degradation process in NMC based cathodes and effect of atomic layer deposited protection layer (such as TiO_2, APO_3), we have used soft and hard XAS in conjunction with other characterization techniques including ultra high-resolution transmission electron microscopy and extensive electrochemical methods. Our results indicate that $AlPO_4$ coated on Li rich NMC cathodes can suppress the oxygen release in these cathodes and increase their columbic efficiency. In addition, $AlPO_4$ compared to Al_2O_3 protection layer, higher positive impact on the thermal stability the cathode material [1].

In the past few years we have employed in-situ XAS methods to study the cathode and anodes of Li ion, Li-S and Na-O_2 batteries during their operation [2-5]. As in example to promote safer high temperature Li-S batteries using carbonate-based electrolyte, we have investigated the reaction processes involved in their cathode electrode in detail. Using in-situ XAS studies we have illustrated the irreversible reactions occurring at the cathode with the application of carbonate electrolyte. Subsequently, we have demonstrated the role of molecular deposited (MLD) alucone coatings as a viable option to address the challenges in carbonate-based Li-S batteries [2]. In addition, we have developed a Na-O_2 cell for in-situ soft XAS measurements, to investigate the formation/decomposition of discharge products in during cycling and study their stability in the cell environment.

These researches demonstrate the crucial role ex-situ and in-situ XAS studies play in development and improvement of energy systems.

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