Application of X-ray Absorption Fine Structures in the Study of Advanced Rechargeable Batteries

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Recently, advanced rechargeable batteries have attracted intensive research attention as one promising solution to solve the global energy and environment problems due to high energy density and long working life, including lithium-ion batteries (LIBs), lithium-sulfur (Li-S) batteries and Alkali metal-oxygen (Li-O_2, Na-O_2) batteries. Although remarkable development has been made on the rechargeable batteries, there are still several challenges for the practical application in electronic vehicles (EVs) and large-scale energy storage. To solve the problems, we applied X-ray absorption fine structures in the study of advanced rechargeable batteries to get a better understanding.

In the case of LIBs, the side reactions occurring at the electrode-electrolyte interface plays the key role in the fast-fading capacity. To overcome the challenge at the interface, we have prepared several ion-conductive layers, such as $FePO_4$, $AlPO_4$, TiO_2, and $LiTaO_3$ on the surface of the lithium nickel manganese oxide (LNMO) and lithium nickel manganese cobalt oxide (NMC) cathode materials to enhance the cycling stability.[1-5] To get a better understanding of the improvement mechanism, XAFS have been applied to study the interface during cycling and indicate that the side reactions have been effectively prevented.

Current Li-S batteries suffer from the commonly-employed ether-based electrolyte due to the low-boiling & flash-points and dissolved polysulfides. To overcome the safety and capacity fading issues, we designed and prepared ultrathin alucone film as an interlayer on carbon-sulfur electrodes through the molecular layer deposition (MLD) method, presenting improved electrochemical performance and realizing stable and high-temperature Li-S batteries in the safe carbonate-based electrolyte. [6,7] To understand the inside mechanism, ex-situ and operando X-ray absorption near edge structure (XANES) study has been applied and indicates that the sulfur cathodes interact with MLD alucone coating and undergoes new electrochemical route in carbonate-based electrolyte.

Li-O_2 and Na-O_2 batteries shows high theoretical energy densities, comparable to the gasoline. However, the practical application is highly hindered by the limited cyclability and high charging overpotential. To get a comprehensive understanding of the electrochemical mechanism and then further design and prepare better Li-O_2 and Na-O_2 batteries, we have applied XANES and Extended X-ray absorption fine structure (EXAFS) to study the electrochemical process and electrode materials.[8-12] Based on the detailed study, the proper solution to realize enhanced electrochemical performance has been pointed out.

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