Probing electrochemical interfaces and solvation in calcium-ion battery using operando soft X-ray spectroscopy

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Synchrotron based X-ray spectroscopic techniques offers unique characterization in many important energy materials of energy conversion, energy storage and catalysis in regards to the functionality, complexity of material architecture, chemistry and interactions among constituents within. However, it is challenging to reveal the real mechanism of the chemical processes. In the operando soft X-ray spectroscopy characterization of interfacial phenomena in energy materials and devices, it has been found that the microstructure and composition of materials as well as the microstructure evolution process have a great influence on performances in a variety of fields, e.g., energy conversion and energy storage materials, chemical and catalytic processes.

The solvation of an electrolyte near the electrolyte/electrode interphase dictates the charge transfer efficiency and therefore affects the performance of a battery. However, current understanding regarding this interphase was limited due to the lack of direct interphase probing approaches under in-situ/operando conditions. In this report, using operando X-ray absorption spectroscopy and resonant soft X-ray scattering through a patterned e-chip, the solvation of a calcium organic electrolyte was investigated under operando conditions. The disruption of the solvation structure by a secondary anion or cation were evaluated using the methodologies developed, which will guide the design of electrolytes for future energy storage. The strategy of these new methodologies developed will also benefit the investigation of catalysis at interphases and electrochemical microenvironments in general.

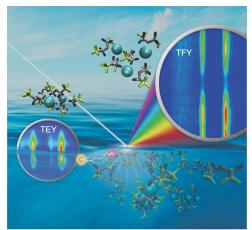


Figure 1. The calcium L-edge XAS spectra, under electrochemically operando conditions in both TEY and TFY modes, provide insights into the calcium solvation structures at the interphase and in the bulk.