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Synchrotron-based X-ray diffraction and spectroscopy for metal-ion battery material studies

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The commercialisation of lithium-ion batteries (LIBs) has gained huge success and LIBs are taking an important part of our daily modern life, as confirmed by the prestigious award of the 2019 Nobel Prize in Chemistry. Owing to the limited abundance of lithium, other metal-ion batteries (MIBs), such as zinc-, sodium-, and potassium-ion batteries, with similar working mechanism, have also been studied and developed as alternatives. Compared with other energy storages, MIBs are relatively less predictable due to the complex reactions occurred on the bulk and surface of electrodes, as well as other battery components, such as electrolyte, during electrochemical processes. During charge and discharge, the intercalation and de-intercalation processes of metal ions (i.e. lithium ions) happening in the electrodes are very complex, involving the evolutions of phase, structure, composition, as well as morphology, with these processes underpinning electrochemical function and performance of the battery. Therefore, a mechanistic understanding of the reaction pathways, i.e. the atomistic and molecular-scale origin of battery performance, will enable the rational improvement of electrode materials and pave the way for entirely new battery systems, and in-situ in-operando synchrotron-based X-ray powder diffraction (XRPD) with high brightness and tuneable wavelength is an extremely powerful tool to obtain this crucial understanding.
On the other hand, X-ray absorption spectroscopy (XAS) could be used to detect the electronic structure of certain ions within the active materials in the battery, especially helpful to investigate the elements with electrochemical activities. Transmission X-ray microscopy (TXM) can be employed to probe the electrode morphological changes during charge and discharge, linking to the electrochemical performance of the materials. Infra-red microscopy (IRM) is also found to be a powerful analytical method, allowing the characterisation of the chemical information and their distribution of solid-electrolyte interphase formed on the electrode surface. By correlating the chemical information with data obtained from other techniques, additional insights into their mechanism, which is critical for further development, can be gained.
In this presentation, I will introduce the research work in our team and showcase some examples of these mechanistic and crystallographic research, demonstrating the important role of synchrotron-based X-ray scattering in battery research.

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