Engineering Better Batteries from the Particle to the Pack

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The Li-ion battery was one of the transformative technologies of the 20th century and promises to have wider impact in the 21st century with the rapid uptake of electric vehicles and the deployment of grid scale energy storage. Energy storage is critical to achieve ambitious targets for Net Zero where electrochemical technologies are expected to be a cornerstone of decarbonisation efforts in a range of sectors. With an increasingly demanding portfolio of applications, there are a suite of emerging battery technologies that can support decarbonisation: alongside developments in advanced Li-ion chemistries, these include solid state, Li-sulfur, sodium and metal-air batteries.

Heterogenous, porous electrodes are common to all of these battery chemistries where the physical morphology of the materials have profound influences on the battery performance. Engineering these materials for energy and power density, lifetime, safety and cost is a challenging, multi-parameter optimisation. Historically, this has been achieved empirically, but with the emergence of advanced modelling and characterisation tools, we are increasingly equipped to rationalise the relationship between microstructure and performance, and to take an informed engineering design approach.

The past decade has seen the rapid development and proliferation of three-dimensional X-ray imaging tools applied to Li-ion batteries. This provides a framework to improve the understanding of electrode morphology and its influence on transport processes, electrochemistry and mechanical behaviour. The non-destructive, and multi-scale characteristics of X-ray imaging tools provide benefits to quantify hierarchical complexity from the particle to the electrode and device level. Moreover, through the application of image-based modelling tools, it has become possible to simulate a range of phenomena using a computational framework derived directly from tomographic images.

Here, we will review this progress and reflect on recent developments using multi-modal methods to understand the performance of advanced batteries. In concert, the portfolio of imaging and modelling tools provides a platform to explore the performance, degradation and failure of Li-ion batteries and to accelerate the development of post Li-ion chemistries.