

Accelerating the understanding of battery materials by integrating first-principles simulations and x-ray and electron characterization

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The understanding, development, and design of battery materials require significant efforts in experimental characterization, especially under operating conditions. While synchrotron x-ray sources and electron microscopes are increasingly able to produce large volumes of data, the interpretation of such data can still be time consuming and difficult, especially in systems with reduced symmetry, such as delithiated battery materials, due to the large number of possible configurations. On the other hand, improvements in first-principles theories, algorithms and computational capabilities have enabled efficient and accurate calculations of battery materials properties from first principles. However, first-principles (e.g. density functional theory (DFT)) modeling requires as inputs atomistic configurations, which are in principle encoded in characterization data. The incorporation of experimental data containing atomic-scale information, such as X-ray diffraction (XRD), X-ray pair distribution function (PDF), X-ray absorption near edge spectra (XANES), and transmission electron microscopy (TEM), with atomistic and first principles computational modeling, can allow the determination of structural evolution in battery materials more efficiently and accurately. In this poster, we will showcase the use of physics-informed machine-learning approaches for experimentally-guided atomistic structure determination, efforts in improving computational predictions of properties and characterization data, and applications towards lithium-ion battery materials including Li-rich cathode materials and solid electrolyte interfaces.