



Pair distribution function analysis of lithium- and sodium-ion battery materials

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Abstract:

Pair distribution function (PDF) analysis is a total-scattering technique; it uses both Bragg scattering and diffuse scattering in parallel to give information both about the local and long-range structure of a material. As it doesn't rely on the presence of long-range order, quantitative information about local structure, e.g. bond lengths, coordination numbers, correlation length or disorder can be determined, even when the material lacks long-range order. High-energy synchrotron X-rays can be used with bespoke electrochemical cells to apply this technique *in operando*; this results in highly consistent data sets at various states-of-charge suitable for detailed analysis. In this talk, some recent structural studies of lithium- and sodium-ion battery materials which use PDF analysis, often in conjunction with other techniques such as powder diffraction and solid-state NMR, will be presented.

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- (3) Jung, H.; Allan, P. K.; Hu, Y.-Y.; Borkiewicz, O. J.; Wang, X.-L.; Han, W.-Q.; Du, L.-S.; Pickard, C. J.; Chupas, P. J.; Chapman, K. W.; Morris, A. J.; Grey, C. P., *Chemistry of Materials*, 2015, 27, 1031

Contribution:

Invited