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Battery cathode crystal structures: seeking to simplify complexity

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The crystallographic analysis of high performance rechargeable batteries is, from a commercial viewpoint, essential for the achievement of optimal performance. From an academic perspective, the precise experimental measurement of these simple pristine materials can pose significant analytical and theoretical challenges.
There is a conundrum at the basis of this research. For example, pristine high-power lithium-ion cathode materials have a very simple crystal structure based on an ordered, layered rock-salt structure. LiCoO2, the prototypic cathode material, adopts a rhombohedral structure with a single variable atomic coordinate; both lithium and cobalt have octahedral moieties. NaCoO2 adopts a similar structure but, on one-third de-intercalation, transitions to a hexagonal symmetry where the oxygen coordination around sodium is trigonal pyramidal.
This talk discusses the challenges of building a simple and accurate model of the crystal structures of sodium-ion battery cathode materials during charging and discharging. Multiple structures have been reported that are based on the octahedral and trigonal-pyramidal prototypes but these structure alone are not sufficient to describe the complexity of the observed powder diffraction data. The approach presented in this talk is based around the analysis of the shearing of neighbouring layers using the minimal number of stacking fault probabilities that precisely model the observed complex powder diffraction patterns.