Tackling the optimisation challenge of structural faulting in battery cathode materials

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The quality of the performance of batteries is directly determined by the atomic-level structure of its constituents: the cathode, anode and electrolyte. The cathode is the most significant battery component as it determines the level of energy capacity and the lifetime battery performance.

This talk focuses on high-performance sodium-ion batteries (SIBs) which complement the success of the lithium-ion battery (LiB). Pristine SIB cathode materials are more complex as a consequence of the ability of sodium to adopt 6-fold oxide coordinated ions, not only in the form of an elongated octahedron (trigonal anti-prism) but also as a trigonal prism; as single phases, the two moieties adopt rhombohedral (O3) and hexagonal (P2) aristotypes respectively.

As a further complication, the small internal energy difference between O3 and P2 structures leads to intergrowths that are determined by the probabilistic appearance of stacking faults. This is crystallographically equivalent to stacking in the simpler graphite/Lonsdalite system and will be briefly explored to identity the principal features of the impact of stacking faults. Fundamental crystallography questions about what is the optimal goodness-of-fit will be discussed.

In addition to the appearance of stacking faults in pristine cathode materials, a rich variety of stacking faults appear during battery charging and discharging. These give deep insights into battery behaviour and performance and offer future directions for improved batteries.