Short-range ordering and degradation processes in cation-disordered lithium transition metal oxide cathodes using solid-state NMR techniques.

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Résumé

Li-ion batteries are a ubiquitous part of modern technology as they provide power to a wide variety of devices, from small portable electronics to electric vehicles, while also providing large-scale storage for the electric grid. Despite their widespread use, Li-ion batteries face some challenges (e.g. use of expensive elements such as Ni and Co, energy density) in order to fulfill their role in the transition from fossil fuel to renewable power source. One promising type of cathode material for Li-ion batteries is based on lithium transition metal oxides with a disordered rock salt structure.[1] These new materials can use Earth abundant elements such as Mn and Ti and can provide higher capacity than their layered transition metal oxides counterpart. Furthermore, these materials can be partially fluorinated, which overall leads to improved electrochemical performance. But structural changes that occur upon fluorination or cycling are difficult to investigate with common long-range scattering techniques, due to the intrinsic disorder on the cation lattice and the impossibility to distinguish F from O. In this regard, solid-state NMR is a powerful local structure probe, which can elucidate short-range order present in these materials and easily distinguish 19F from 17O. Here, examples of our work will illustrate how solid-state NMR can allow one to unravel structure-property relationships that can then lead to the rational design of cathode materials with enhanced performance. [1] R. J. Clément, Z. Lun and G. Ceder, Energy Environ. Sci., 2020, 13, 345-373.

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