Structural and electrochemical investigations of fluorine doped $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$

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Lithium-ion batteries (LIBs) are considered to be the key technology in pushing electric vehicles (EV) to the consumer market due to their high gravimetric and volumetric energy density. Nevertheless, in LIBs must fulfil many crucial criteria in order to be truly marketable (e.g. fast charging times, a comparable driving range to combustion engines and small packaging size). However, achieving this goal first requires the optimization of the LIB components, such as the separator, the anode and the cathode. As such, many studies have focused on the optimization of $Li_{1+a}(Ni_{1-x-y}Co_xMn_y)_{1-a}O_2$ (NCM) cathode material. Notably, employing higher nickel fractions allow for higher capacities due to better lithium utilization. Unfortunately, the structural and electrochemical stabilities suffer at higher nickel fractions, which in turn leads to poor cycle life, low thermal stability and added safety risks. To mitigate the aforementioned issues, the incorporation of various dopants has emerged as a promising strategy. There are two different ways of doping (i) cation doping and (ii) anion doping. While cation doping is more widely used, anion doping provides the opportunity for enhancing the electrochemical properties without sacrificing the electrochemically active elements.

Herein, fluorine has been used as anionic dopant in NCM toward enhancing the associated electrochemical and structural properties. The impact on the structure was investigated by Rietveld and pair distribution function analysis of total scattering data. The measurements revealed a variation of the interslab distance, which is known to influence electrochemical performance by altering the activation energies for lithium diffusion.[1] Moreover, EDX, XPS and ToF-SIMS were employed to probe the efficacy of dopant incorporation within the layered NCM structure. Only the surface of the fluorine doped NCM particles contained fluoride species. The fluoride surface layer reduces the transition metals at the subsurface, resulting in a continuous variation of the lattice parameters form the core out toward the surface. Additionally, the electrochemical performance of the doped materials was investigated by galvanostatic cycling. The fluorine doped NCM exhibited lower capacities, but higher cycling stability relative to the pristine material.

References:

[1] K. Kang, G. Ceder, Factors that affect Li mobility in layered lithium transition metal oxides. *Phys. Rev. B* **2006**, *74*.