Na-doped Method of Layered Li$_{1.2}$Mn$_{0.54}$Ni$_{0.13}$Co$_{0.13}$O$_2$ for High Capacity and High-rate Li-ion Batteries

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High energy and power-density lithium-ion batteries (LIBs) are critically needed for applications in aerospace, EVs, energy storage systems and so on\cite{1}. Lack of high performance cathode materials has become a technological bottleneck for the commercial LIBs. Due to the high reversible capacity (300mAh/g), layered Li$_{1.2}$Mn$_{0.54}$Ni$_{0.13}$Co$_{0.13}$O$_2$ has been paid much attention\cite{2}. Despite its high specific capacity, Li$_{1.2}$Mn$_{0.54}$Ni$_{0.13}$Co$_{0.13}$O$_2$ suffers poor rate capability, which was ascribed to two-dimensional ion channel caused by layered structure. Moreover, layered Li$_{1.2}$Mn$_{0.54}$Ni$_{0.13}$Co$_{0.13}$O$_2$ has irreversible structural rearrangement above 4.5V during the first charge process. The irreversible capacity loss is due to the oxidation of O$^{2-}$ ions, which involves the extraction of lithium as Li$_2$O during first charge process and the inability to insert part of the extracted lithium back into the lattice during the first discharge process\cite{3}. Many efforts have been devoted to address these challenges.

Here we report a reasonable design and synthesis of cathode material. Na-doped Li$_{1.2}$Mn$_{0.54}$Ni$_{0.13}$Co$_{0.13}$O$_2$ has been synthesized by high-temperature solid-state molten salt method for the first time. Our results indicate that Na$^+$ ion enters the lattice instead of the Li$^+$ ion with no change the structure. Compared to pristine sample, Na-doped sample has excellent rate and capacity performance, and the irreversible capacity loss decreases from 75 to 40mAh/g. The performance improvements are responsible for the larger ion radius of Na$^+$ ion (102pm) than that of Li$^+$ ion (76pm), as shown in Fig.1. Due to a proper amount of sodium is substituted for the position of lithium, the Li$^+$ ion diffusion channel of the 2D layered structure is expanded, which is beneficial to the lithium ions insertion/extraction reaction. At the same time, the oxygen vacancy can be reduced above 4.5V, which reduces the irreversible loss and improves the stability of the material.

![Fig.1 Schematic of Na doping in Li$_{1.2}$Mn$_{0.54}$Ni$_{0.13}$Co$_{0.13}$O$_2$ material.](image)

References: