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# PROGRAMME AND THE BOOK OF ABSTRACTS

3rd International Symposium on Materials for Energy Storage and Conversion - mESC-IS 2018

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# Fluorination of sodium cobalt oxide: effects on structure and electrochemical performance

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Lower market cost of sodium in contrast to lithium makes sodium intercalating compounds attractive for application as electrodes in rechargeable sodium batteries. Among them, sodium cobalt oxide, $Na_xCoO_2$, have been extensively investigated as potential cathode material for sodium ion batteries [1]. $Na_xCoO_2$ crystallizes in a number of layered structures depending on sodium content, oxygen partial pressure and temperature [2]. In each of these structures, edge-sharing $CoO_6$ octahedra form sheets between which sodium ions are inserted with trigonal prismatic (P) or octahedral (O) environment. The packing differs in the number of sheets within the unit cell – 2 or 3 sheets – creating three possible structural types denoted as O3, P2, and P3. The P2 type of structure (displayed in Figure 1) is considered as the most suitable for electrochemical application for its cycle stability.

Within this research the possibility of fluorine doping of the P2 type $Na_xCoO_2$ powder was examined. As fluorine substitution already proved successful in improving cathode performance of layered lithium-based counterparts, the effects of fluorination on structure and electrochemical properties of P2 $Na_xCoO_2$ were investigated and discussed.

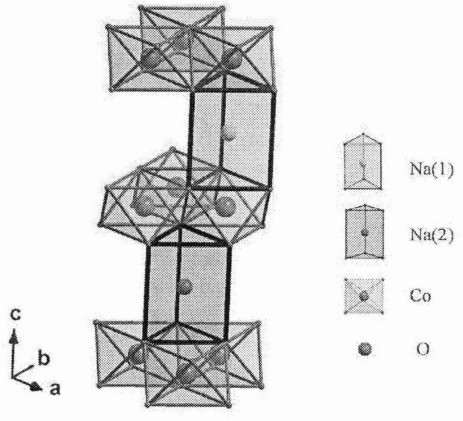


Figure 1. P2 structure of $Na_xCoO_2$.

A modified solid state reaction (an adopted method that includes sequential cycles of rapid heating – at 750°C in the air with dwell time of 15 minutes – and rapid cooling, with an intermediate grinding of the powder between two cycles) was applied for the preparation of a pristine $Na_xCoO_2$ powder. $Na_2CO_3$ and $Co_3O_4$ in a molar ratio 1.7 : 1 were used as starting compounds. Fluorination of the synthesized $Na_xCoO_2$ has been conducted at 200 °C in a vacuum evacuated atmosphere with $NH_4HF_2$ as a fluorination agent. The obtained samples were analysed by X-ray powder diffraction, FTIR spectroscopy, FESEM electron microscopy, X-ray photoelectron spectroscopy and Galvanostatic charge/discharge tests.

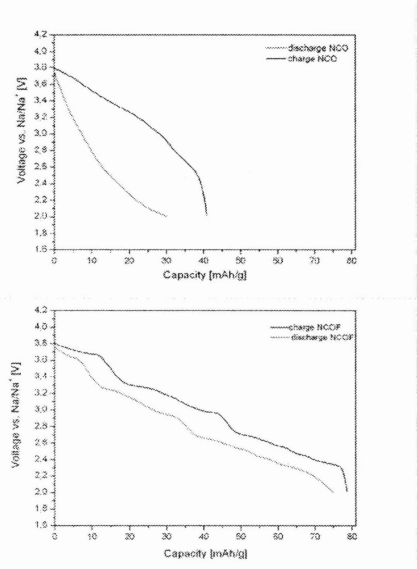


Figure 2. Galvanostatic charge/discharge profiles for pristine (upper graph) and fluorinated powder (lower graph).

The results of the Rietveld refinement combined with the findings from the X-ray photoelectron spectroscopy measurements confirm $Na_{0.76}CoO_2$ and $Na_{0.44}CoO_{1.96}F_{0.04}$ stoichiometries for the pristine and fluorinated powders, respectively, which implies that 4 at.% of fluorine ions per formula unit are incorporated in the structure. Fluorination modifies the structure through both the reduction of crystallite size and the increase of interslab distance. Consequently, fluorinated powder has showed the improvement of the electrochemical performances (Figure 2).

**References**

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