Accepted Manuscript

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PII: S0925-8388(18)33533-3

DOI: 10.1016/j.jallcom.2018.09.281

Reference: JALCOM 47700

To appear in: *Journal of Alloys and Compounds*

Received Date: 13 July 2018

Revised Date: 16 September 2018

Accepted Date: 23 September 2018

Please cite this article as: M. Zhang, H. Zhao, M. Tan, J. Liu, Y. Hu, S. Liu, X. Shu, H. Li, Q. Ran, J. Cai, X. Liu, Yttrium modified Ni-rich $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ with enhanced electrochemical performance as high energy density cathode material at 4.5□V high voltage, *Journal of Alloys and Compounds* (2018), doi: https://doi.org/10.1016/j.jallcom.2018.09.281.

Yttrium modified Ni-rich $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ with enhanced electrochemical performance as high energy density cathode material at 4.5 V high voltage

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Abstract: This work adopts an effective method to stabilize the structure of Ni-rich $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ with yttrium modifying. The results of XRD, EDS, HR-TEM and XPS tests verify that the yttrium modified materials integrate surface nanoscale $LiYO_2$ coating and inner gradient Y^{3+} doping. TGA and DSC tests confirm that yttrium modification can promote the thermal stability of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ cathode material. The results of galvanostatic charge-discharge tests suggest that the 2 mol % yttrium modified sample can exhibit a superior cycling performance with initial discharge capacity of 189.4 mAh g^{-1} and outstanding capacity retention of 98.4% after 100 cycles at 2.8-4.5V, which presents obvious enhancement compared with the 83.5% capacity retention of pristine sample. The cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) tests indicate that 2 mol % yttrium modifying significantly enhances the diffusion of Li^+ ions (D_{Li}^+) and notably decreases the electrochemical polarization of electrodes. The surface Li-ion conductor $LiYO_2$ coating layer as a surface protector inhibits the side reaction and the gradient Y^{3+} doping supports the crystal structure, which can show synergistic effect in enhancing the electrochemical performance of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ cathode material.

Keywords: Ni-rich cathode, Yttrium modification, $LiYO_2$, Gradient doping, High voltage

1. Introduction

Ni-rich layered cathode materials are considered as the most likely candidate of

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