Accepted Manuscript

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PII: S0013-4686(18)31664-5

DOI: 10.1016/j.electacta.2018.07.149

Reference: EA 32346

To appear in: *Electrochimica Acta*

Received Date: 8 May 2018

Revised Date: 19 July 2018

Accepted Date: 20 July 2018

Please cite this article as: L. Wang, L. Deng, Y. Li, X. Ren, H. Mi, L. Sun, P. Zhang, Y. Gao, Nb^{5+} doped LiV_3O_8 nanorods with extraordinary rate performance and cycling stability as cathodes for lithium-ion batteries, *Electrochimica Acta* (2018), doi: 10.1016/j.electacta.2018.07.149.

Nb^{5+} Doped LiV_3O_8 nanorods with extraordinary rate performance and cycling stability as cathodes for Lithium-ion batteries

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Abstract

Cathode materials are the key component and bottleneck that hinders the development of lithium-ion batteries. This work reports the preparation of LiV_3O_8 nanorods with different levels of Nb doping through a sol-gel process and a subsequent electrospinning method. The electrochemical performance of LiV_3O_8 as a cathode material was enhanced significantly upon Nb doping. A capacity of 401 mAh g^{-1} at 0.1 C (0.52 mAh cm^{-2}) was observed for $LiV_{2.94}Nb_{0.06}O_8$, which still retained a value of 91 mAh g^{-1} (0.12 mAh cm^{-2}) at 20 C.. The doped cathode also showed excellent cycling stability, retaining 99.7% of its initial capacity after 500 cycles of charge and discharge. The mechanisms for the performance enhancement were investigated using experimental techniques and theoretical analysis based on density functional theory (DFT). It was found the Nb doping could expand the lattice space, reduce the bandgap, increase the intrinsic conductivity, lower the energy barrier of the reaction and