

Author's Accepted Manuscript

Iron Migration and Oxygen Oxidation during
Sodium Extraction from NaFeO_2

Yejing Li, Yurui Gao, Xuefeng Wang, Xi Shen,
Qingyu Kong, Richeng Yu, Gang Lu, Zhaoxiang
Wang, Liquan Chen



PII: S2211-2855(18)30136-8
DOI: <https://doi.org/10.1016/j.nanoen.2018.03.007>
Reference: NANOEN2555

To appear in: *Nano Energy*

Received date: 13 December 2017
Revised date: 6 February 2018
Accepted date: 2 March 2018

Cite this article as: Yejing Li, Yurui Gao, Xuefeng Wang, Xi Shen, Qingyu Kong, Richeng Yu, Gang Lu, Zhaoxiang Wang and Liquan Chen, Iron Migration and Oxygen Oxidation during Sodium Extraction from NaFeO_2 , *Nano Energy*, <https://doi.org/10.1016/j.nanoen.2018.03.007>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Iron Migration and Oxygen Oxidation during Sodium Extraction from NaFeO₂

Yejing Li,^{1,2} Yurui Gao,^{1,3} Xuefeng Wang,^{1,4} Xi Shen,⁵ Qingyu Kong,⁶ Richeng Yu,^{2,5} Gang Lu,³
Zhaoxiang Wang,^{*1,2} Liquan Chen¹

1. Key Laboratory for Renewable Energy, Chinese Academy of Sciences; Beijing Key Laboratory for New Energy Materials and Devices; Beijing National Laboratory for Condensed Matter Physics; Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100190, China

2. School of Physical Sciences, University of Chinese Academy of Sciences, P. O. Box 603, Beijing 100190, China

3. Department of Physics and Astronomy, California State University Northridge, Northridge, California 91330-8268, USA

4. Department of NanoEngineering, University of California San Diego, 9500 Gilman Drive, La Jolla, California 92093, USA

5. Laboratory for Advanced Materials & Electron Microscopy, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100190, China

6. Synchrotron Soleil, L'Orme des Merisiers St-Aubin, 91192 Gif-sur-Yvette Cedex, France

The abundant resource of sodium (Na) makes the Na-ion batteries a promising alternate to the Li-ion batteries in electric energy storage, especially when iron (Fe)-based oxide electrodes are used. Layer-structured Na_xFe_yM_{1-y}O₂ (*M* for Mn and Ni, *etc.*), for example, has drawn much attention and is one type of the most attractive cathode materials for the Na-ion batteries. However, the poor cycling performance hinders their applications and the underneath mechanism for their poor performances remains unclear. In this study, the structural transition of NaFeO₂ was characterized and the driving forces for the irreversible Fe migration and O oxidation were explored during Na extraction. The Fe migration from the Fe layer to the Na layer was observed for the first time at the atomic scale. The chemical states and coordination environment of the Fe ions within the Na layer were determined. The density functional theory (DFT) calculations were carried out to understand the Fe migration and O oxidation. These findings provide helpful revelation on constructing the structure and improving the performance of the NaFeO₂-structured cathode materials for the Na-ion batteries.

Keywords: NaFeO₂, iron migration, oxygen oxidation, structural evolution, layered oxides, Na ion batteries

1. Introduction

The importance of the O3-NaFeO₂ ($R\bar{3}m$) structured materials cannot be overstated for either the Li- and Na-ion batteries (LIBs and NIBs).[1, 2] The basic structure of these materials is composed of slabs of edge-shared MO₆ octahedrons, between which are located the alkali (Li or Na) ions.[3] Many of the well-known cathode materials can actually be regarded as their derivatives, such as LiCoO₂ the most classical material for the LIBs,[4] $x\text{Li}_2\text{MnO}_3\cdot(1-x)\text{LiMO}_2$ ($0 < x < 1$, *M* for transition metals) the well-known high-capacity Li-rich materials for the next-generation LIBs,[5] LiNi_xMn_yCo_{1-x-y}O₂ for the LIBs in the electric vehicles,[6] and Na_xMO₂ ($0.67 \leq x \leq 1$) for the NIBs.[7] However, extraction of the alkali ions generates vacancies in the Li or Na layer, to which the transition metal (TM) ions are prone to migrate, resulting in irreversible structural degradation and deteriorated electrochemical performances of some of these oxides.

Download English Version:

<https://daneshyari.com/en/article/7952762>

Download Persian Version:

<https://daneshyari.com/article/7952762>

[Daneshyari.com](https://daneshyari.com)