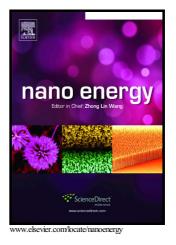
## Author's Accepted Manuscript

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## **ACCEPTED MANUSCRIPT**

## Iron Migration and Oxygen Oxidation during Sodium Extraction from NaFeO2

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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<sub>x</sub>Fe<sub>y</sub> $M_{1-y}O_2$  (*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 NaFeO<sub>2</sub> 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 NaFeO<sub>2</sub>-structured cathode materials for the Na-ion batteries.

Keywords: NaFeO<sub>2</sub>, iron migration, oxygen oxidation, structural evolution, layered oxides, Na ion batteries

## 1. Introduction

The importance of the O3-NaFeO<sub>2</sub> ( $R\bar{3}m$ ) 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 MO<sub>6</sub> 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 LiCoO<sub>2</sub> the most classical material for the LIBs,[4]  $xLi_2MnO_3 \cdot (1-x)LiMO_2$  ( $0 \le x \le 1$ , M for transition metals) the well-known high-capacity Li-rich materials for the next-generation LIBs,[5] LiNi<sub>x</sub>Mn<sub>y</sub>Co<sub>1-x-y</sub>O<sub>2</sub> for the LIBs in the electric vehicles,[6] and Na<sub>x</sub> $MO_2$  ( $0.67 \le x \le 1$ ) 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.

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