

# **Fundamental Understanding the Relationship Between Oxygen Vacancies and Structure Degradation for Cathode Materials in Lithium-Ion Batteries**

Wooyoung Jin<sup>a</sup>, Sanghan Lee<sup>a</sup>, Ilyong Kim<sup>a</sup>, Jaephil Cho<sup>\*a</sup>

<sup>a</sup> *Department of Energy Engineering and School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan 689-798, South Korea*

E-mail: jpcho@unist.ac.kr

Lithium ion batteries (LIBs), which is an electrochemical energy storage, not only is safe and eco-friendly, but also effectively generates electrical energy compared to other energy storage system. In order to develop a battery system, it is necessary to overcome the current limit of LIBs and it requires a sufficient understanding of capacity fading. General reasons for capacity fading of LIBs cathode materials are structure degradation, transition metal dissolution, micro-crack formation in a single crystal, and loss of electronic conductivity caused by particle pulverization. Although many studies have been carried out, most cases have been observed phenomenon rather than the fundamental understanding of capacity fading. In this study, we focused on investigation of the relationship between oxygen vacancy and structure degradation of lithium transition metal oxides. Among LIBs cathode materials, spinel structure of oxygen deficient  $\text{LiMn}_2\text{O}_4$ , layered structure of  $\text{LiCoO}_2$  and  $\text{LiNi}_x\text{Co}_y\text{Mn}_z\text{O}_2$  are prepared. Then, their structure changes after cycling at elevated temperature were analyzed by high-resolution transmission electron microscopy (HR-TEM), X-ray diffraction (XRD), and supported by computational studies. Herein, we have demonstrated that structure degradation of LIBs cathode materials can be started from the inside of a single crystal because of an unavoidable existence of oxygen vacancies in metal oxide and their diffusion and condensation toward the specific plane.