

Supporting Information for  
Why is the O3 to O1 phase transition hindered in LiNiO<sub>2</sub> on full  
delithiation?

Naohiro Ikeda<sup>1</sup>, Itsuki Konuma<sup>1</sup>, Hongahally Basappa Rajendra<sup>2</sup>, Taira Aida<sup>3</sup>,  
and Naoaki Yabuuchi<sup>1, 2, 4\*</sup>

<sup>1</sup>Department of Chemistry and Life Science, Yokohama National University, 79-5 Tokiwadai,  
Hodogaya-ku, Yokohama, Kanagawa 240-8501, Japan

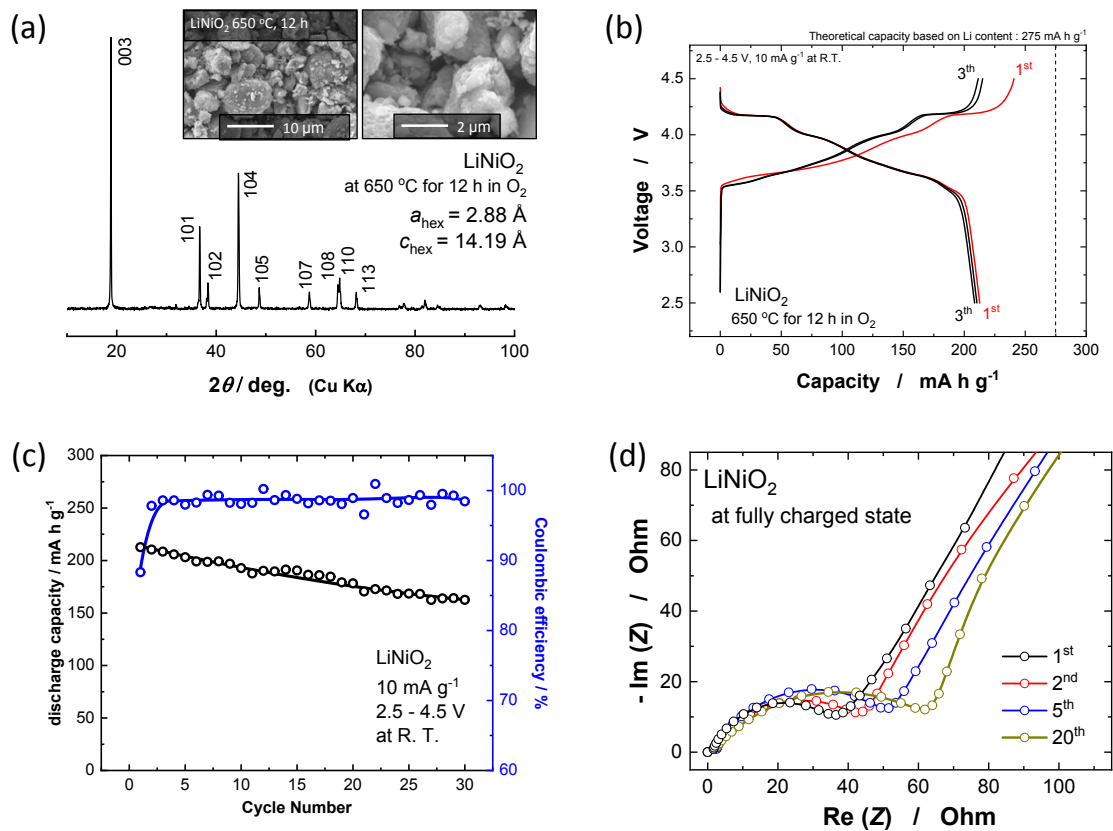
<sup>2</sup>Advanced Chemical Energy Research Center, Yokohama National University, 79-5 Tokiwadai,  
Hodogaya-ku, Yokohama, Kanagawa 240-8501, Japan

<sup>3</sup>Sumitomo Metal Mining Co., Ltd., Battery Research Laboratories, 17-3, Isoura-cho, Nihama,  
Ehime 792-0002, Japan

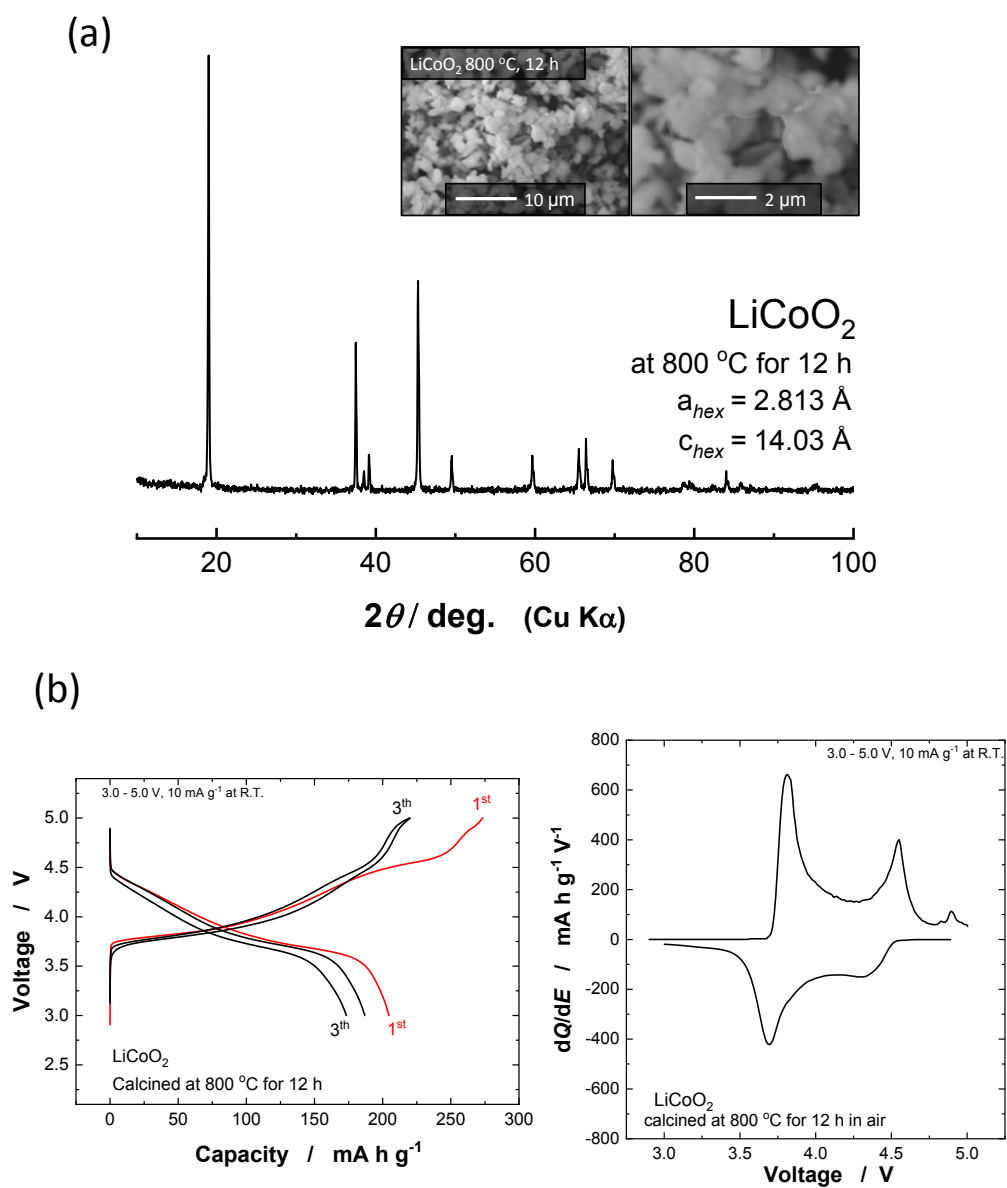
<sup>4</sup>Elements Strategy Initiative for Catalysts and Batteries, Kyoto University, f1-30 Goryo-Ohara,  
Nishikyo-ku, Kyoto 615-8245, Japan

\*corresponding author, e-mail: yabuuchi-naoaki-pw@ynu.ac.jp

## Supporting Figures



**Figure S1.** (a) An XRD pattern and SEM image and (b) charge/discharge curves of  $\text{LiNiO}_2$  used in this study. Discharge capacity retention and Coulombic efficiency for 30 cycles are also shown in (c). (d) Changes in the impedance of  $\text{LiNiO}_2$  at fully charged state.



**Figure S2.** (a) An XRD pattern and SEM image and (b) charge/discharge curves with differential capacity plots of LiCoO<sub>2</sub> used in this study.

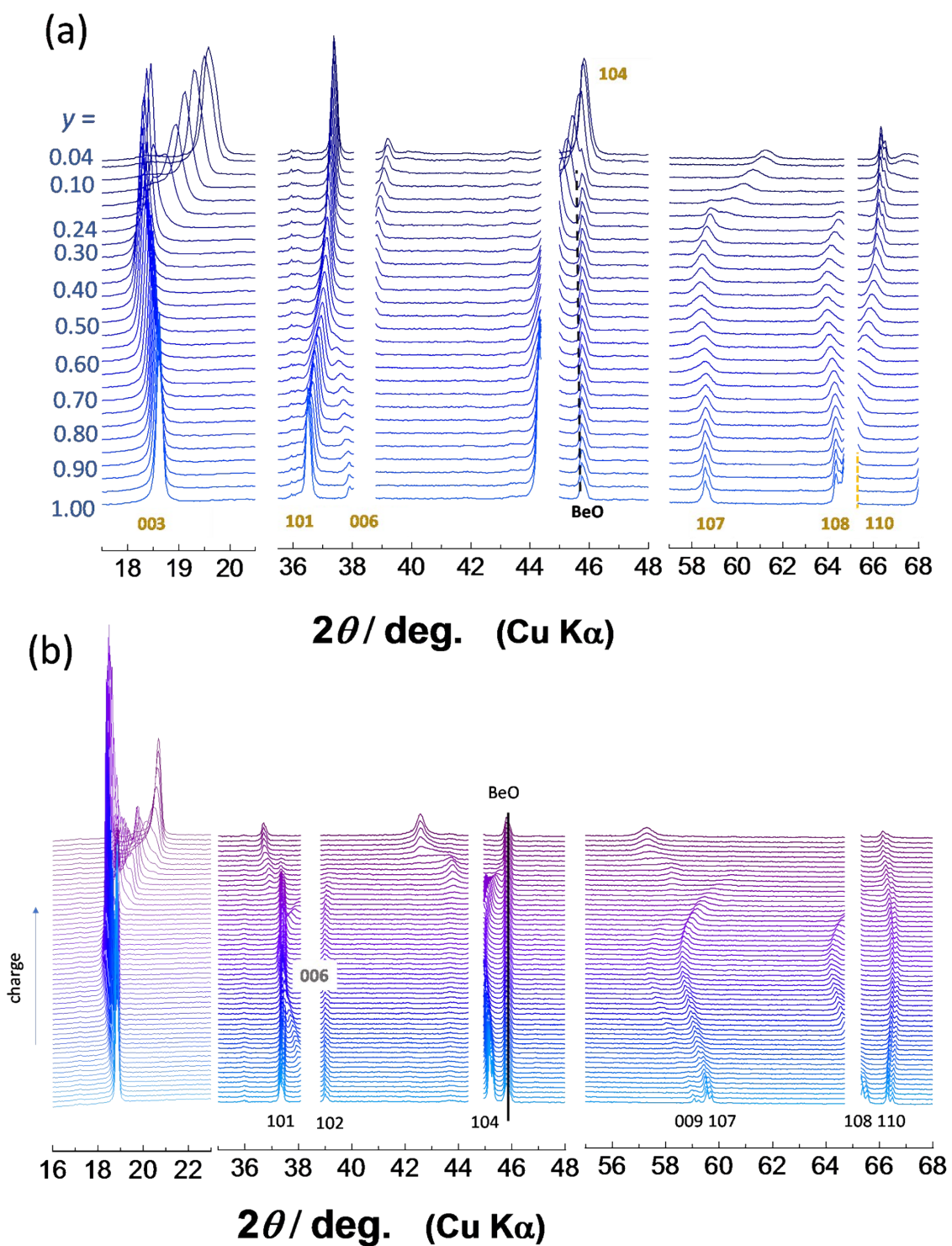
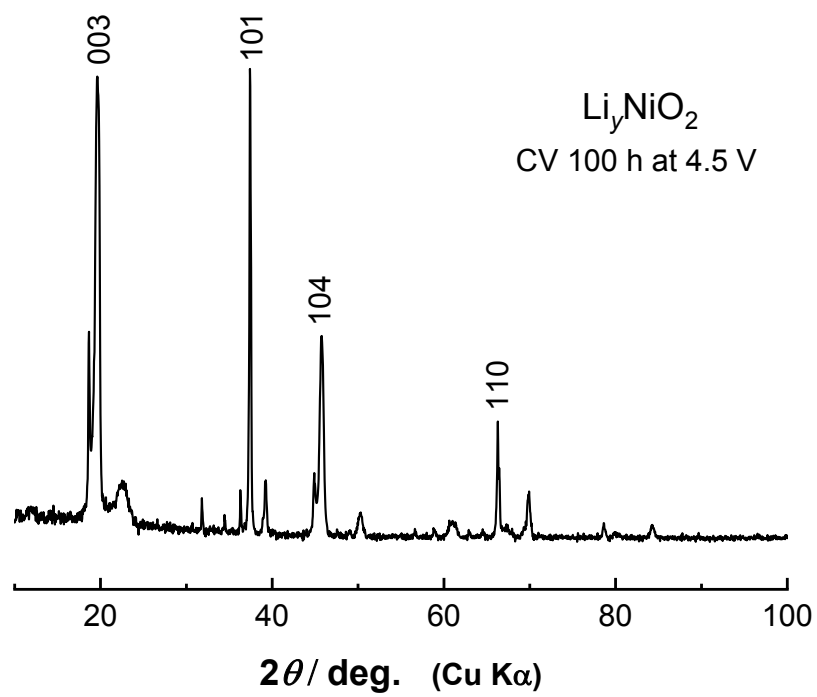
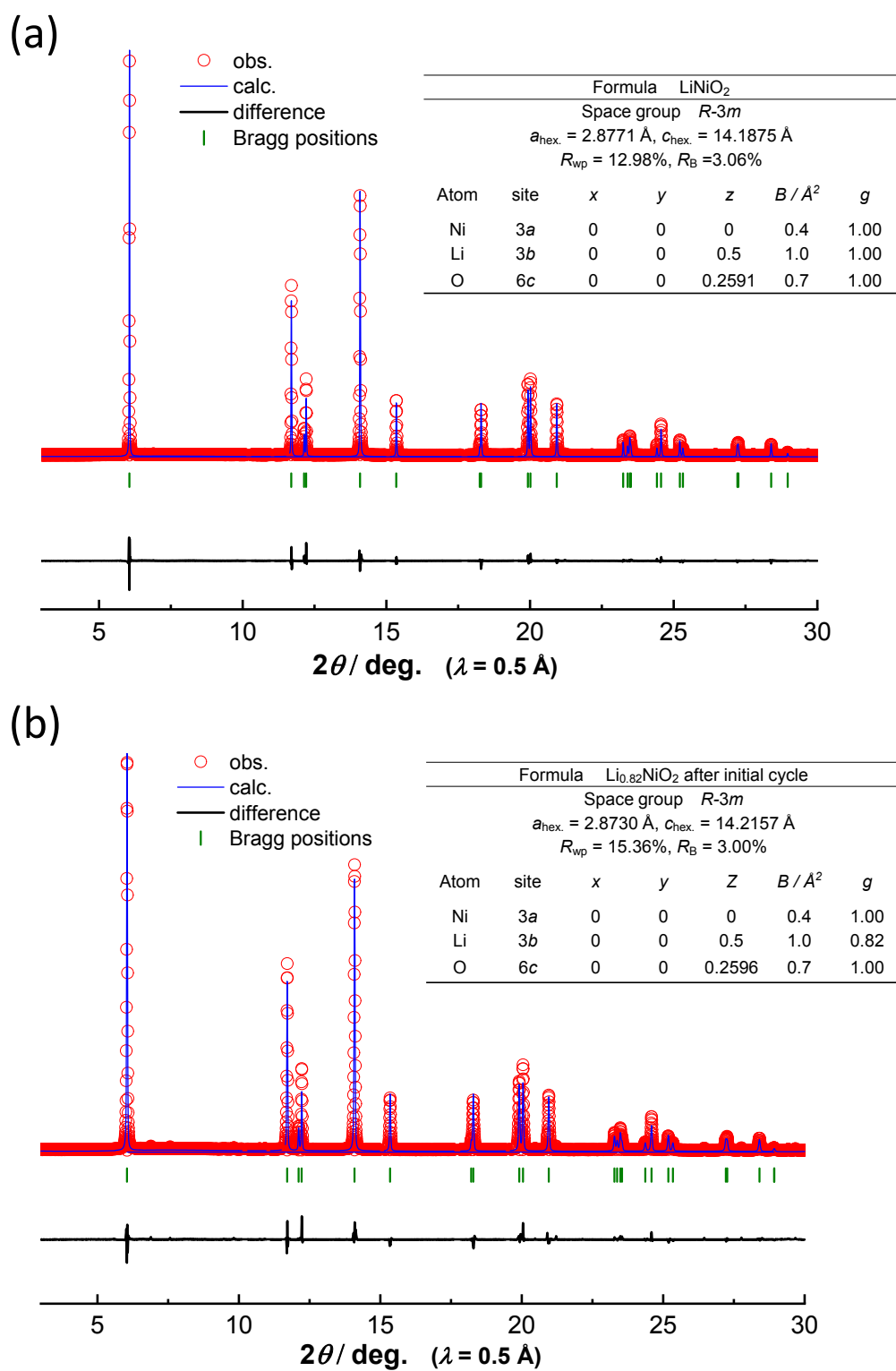


Figure S3. *In-situ* XRD patterns of (a)  $\text{LiNiO}_2$  and (b)  $\text{LiCoO}_2$  at a rate of  $5 \text{ mA g}^{-1}$ .



**Figure S4.** An XRD pattern of  $\text{NiO}_2$  obtained by voltage holding at 4.5 V for 100 h in a Li cell.



**Figure S5.** Results of Rietveld analysis on as-prepared LiNiO<sub>2</sub> (a) and Li<sub>0.82</sub>NiO<sub>2</sub> after the initial cycle (b).