Supporting Information

Li_2NbHO_2: a new transition-metal oxyhydride with rock-salt-type structure

Fumitaka Takeiri,[a,b] Keiko Kusumoto,[a,c] Kosuke Kawai,[d] Hiroshi Yaguchi,[a] Takashi Saito,[e] Kazuhiro Mori,[e] Saburo Hosokawa,[f] Masashi Okubo,[d] Genki Kobayashi*[a,d]

*Corresponding author

genki.kobayashi@riken.jp (Genki Kobayashi)

[a] *Solid State Chemistry Laboratory, Cluster for Pioneering Research (CPR), RIKEN, Saitama 351-0198, Japan*

[b] *Department of Chemistry, Kindai University, Osaka 577-8502, Japan*

[c] *Department of Structural Molecular Science, School of Physical Sciences SOKENDAI (The Graduate University for Advanced Studies), Aichi 444–8585, Japan*

[d] *Department of Chemistry, Electrical Engineering and Bioscience, Waseda University, Tokyo 169-8555, Japan*

[e] *Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Ibaraki 305-0801, Japan*

[f] *Faculty of Materials Science and Engineering, Kyoto Institute of Technology, Kyoto 6068585, Japan*

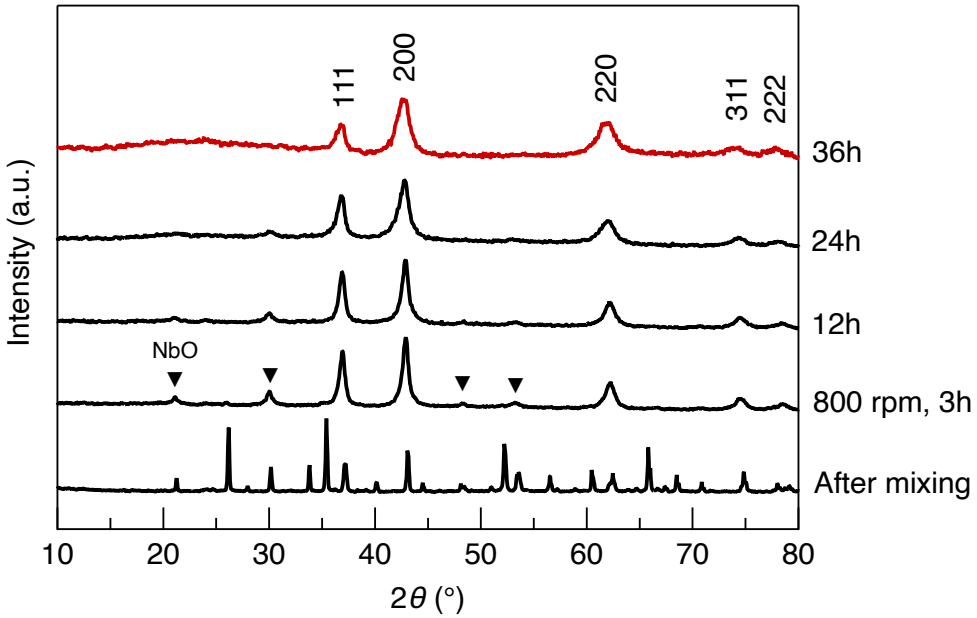

Figure S1. X-ray diffraction patterns of raw materials after hand-mixing and obtained powders by ball milling at 800 rpm for several reaction time.

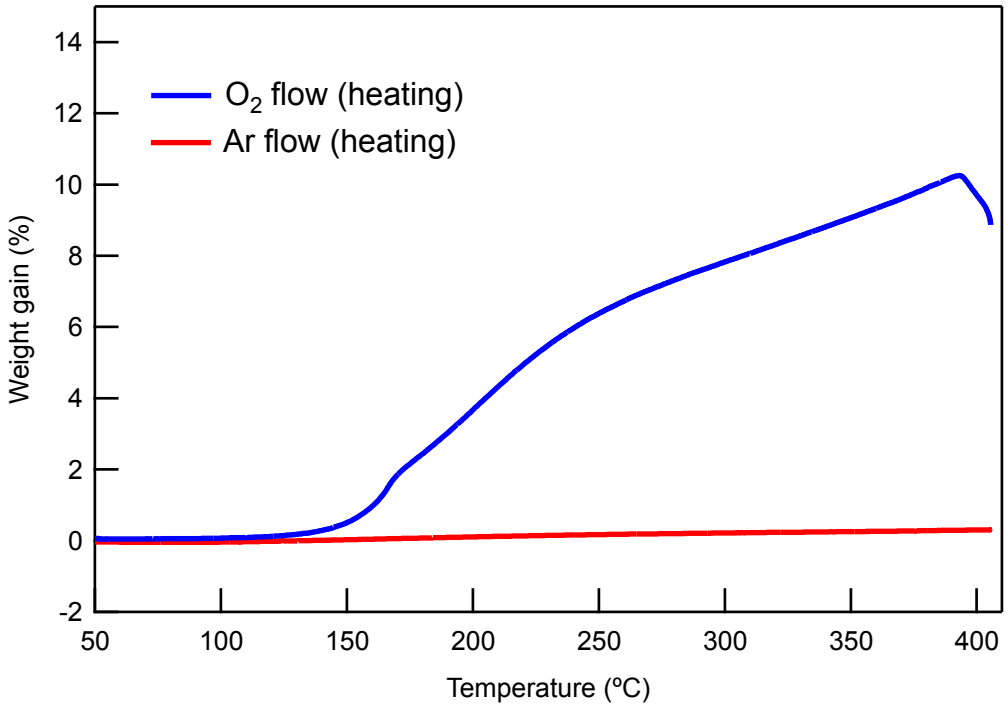

Figure S2. Thermogravimetric data of Li_2NbHO_2 under O_2 and Ar gas flowing at 100 mL·min^{-1}, using a Rigaku Thermo Plus II apparatus.

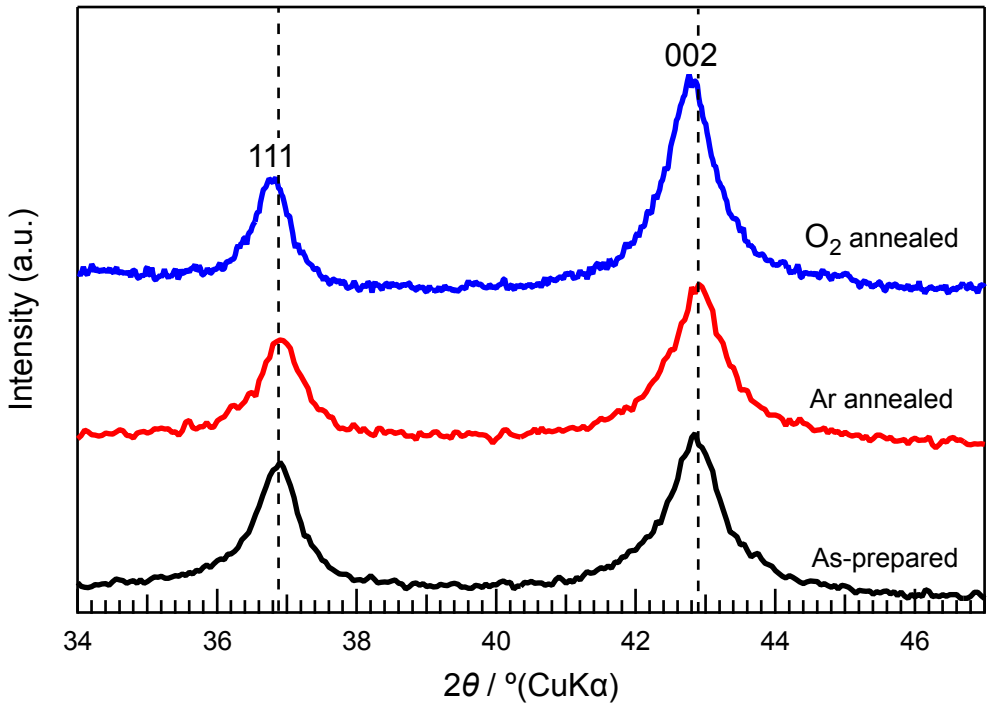

Figure S3. X-ray diffraction patterns of Li_2NbHO_2 before and after TG measurements.

As shown in Fig. S2, a weight gain suggesting ion exchange between H^- and O^{2-} was detected from approximately 125 °C under dry O_2 gas flow, while no significant weight gain was observed under Ar flow. In addition to comparing the XRD patterns before and after the TG measurements (Fig. S3), there was no significant change after the measurement under Ar atmosphere, whereas a significant peak shift to lower angles while maintaining symmetry was observed after the measurement under dry O_2 atmosphere, implying an anion exchange reaction from H^- to O^{2-}. These results indicate that Li_2NbHO_2 is stable at battery operating temperatures and atmospheres.