

Supporting Information

Highly Swollen Layered Nickel Oxide with a Trilayer Hydrate Structure

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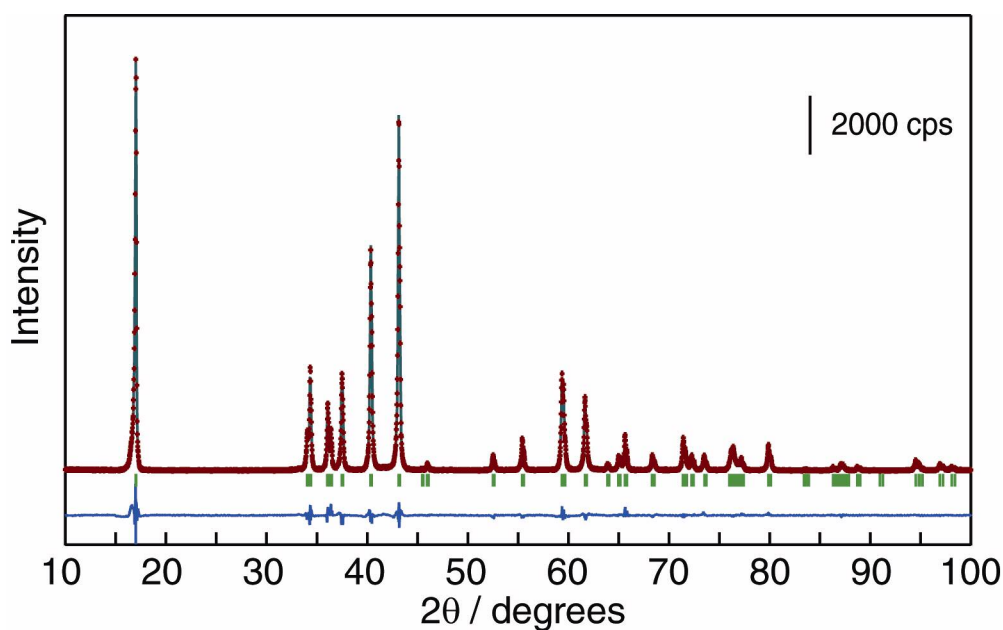


Figure S1. Rietveld refinement pattern for NaNiO_2 . Observed (crosses), calculated (smooth line) and their difference (blue trace). The tick marks indicate the positions of allowed Bragg reflections.

Table S1. Structure Parameters of NaNiO_2

Atom	Wyckoff index	Occupancy	x	y	Z	$U/\text{\AA}^2$
Ni	2a	1	0	0	0	0.0099(4)
O	4i	1	0.2829(4)	0	0.8035(4)	0.0107(7)
Na	2d	1	0	$\frac{1}{2}$	$\frac{1}{2}$	0.0165(7)

*¹Space group: $C2/m$ (No. 12)

*² $a = 5.3222(3) \text{ \AA}$, $b = 2.8458(1) \text{ \AA}$, $c = 5.5832(3) \text{ \AA}$, $\beta = 110.474(3)^\circ$, $V = 79.221(7) \text{ \AA}^3$; $R_{wp} = 11.57\%$, $R_p = 7.70\%$, $R_B = 1.89\%$, $R_F = 1.17\%$, $R_R = 8.99\%$, $S = 1.76$

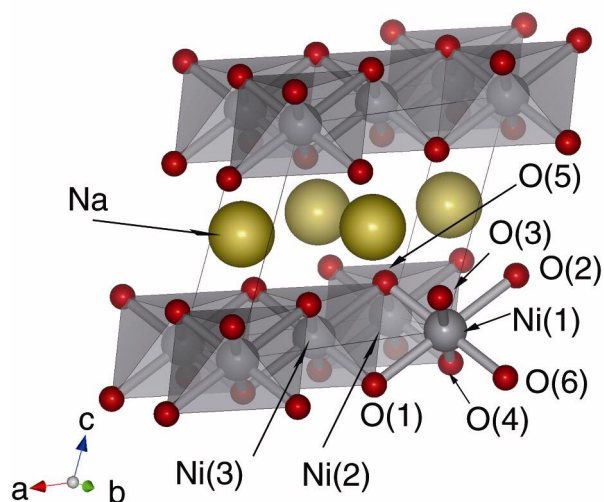


Figure S2. Crystal Structure for NaNiO_2 . Selected interatomic distances (in Å): Ni(1)–O(1) and Ni(1)–O(2) 2.151(2); Ni(1)–O(3), Ni(1)–O(4), Ni(1)–O(5) and Ni(1)–O(6) 1.9176(9); Ni(1)–Ni(2) 2.84580(9); Ni(1)–Ni(3) 3.01763(13).

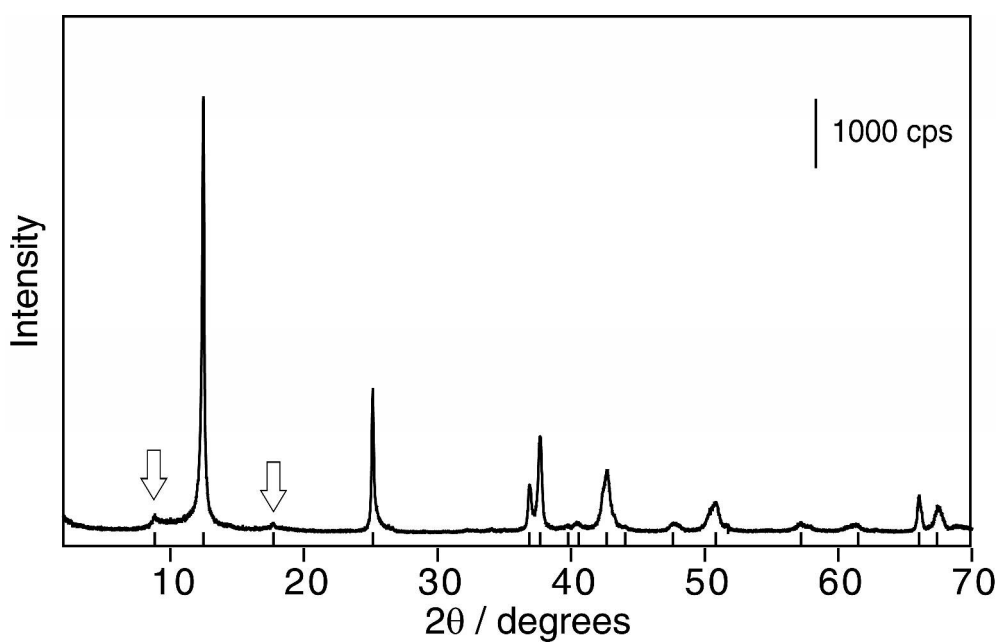


Figure S3. XRD data for a sample obtained after treating the γ -phase, $\text{Na}_{0.33}\text{NiO}_2 \cdot 0.5\text{H}_2\text{O}$, with pure water. The reflections indicated by an arrow indicate the formation of a 10 Å phase in a small amount. The other peaks remained unchanged during the treatment with water and are attributable to the original γ -phase structure.