Phase transition behavior of NaCrO₂ during sodium extraction studied by synchrotron-based X-ray diffraction and absorption

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Fig. S1 Synchrotron diffraction pattern of NaCrO₂ and Rietveld refinement of its structure. The experimental (blue circles) and the calculated (black line) X-ray diffraction patterns are in good agreement with the smooth difference line (red line). The space group is R-3m. The calculated lattice parameters are: a=b=2.9768(6) Å, c=16.9895(3) Å.
Fig. S2  SEM image of the pristine NaCrO₂ powder.
Ex-situ synchrotron x-ray diffraction pattern of the fully charged NaCrO$_2$ (~Na$_{0.5}$CrO$_2$) and Rietveld refinement of its structure. The experimental (blue circles) and the calculated (black line) X-ray diffraction patterns are in good agreement with the smooth difference line (red line). It was indexed with a monoclinic cell (space group: C2/m) with the following parameters: \(a_M (~\sqrt{3} a_R) = 5.0178(7) \, \text{Å}, b_M (~b_R) = 2.8828(3), c_M (~c_R/3\sin\beta) = 5.9027(5) \, \text{Å}, \beta = 106.97^\circ\).
Fig. S4 Schematic for the relative position between Cr and Na ions in Na$_{1-x}$CrO$_2$ at different charge state (x=0, 0.25, 0.5). It corresponds to the Na coordination evolution from octahedral to pseudo-tetrahedral, then to trigonal-prismatic.