Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Phase transition behavior of $NaCrO_2$ during sodium extraction studied by synchrotron-based X-ray diffraction and absorption

Yong-Ning Zhou,[a] Jing-Jing Ding,[b] Kyung-Wan Nam,[a] Xi-Qian Yu,[a] Seong-Min Bak,[a] En-Yuan Hu,[a] Jue Liu,[a] Jian-Ming Bai, [a] Hong Li,[c] Zheng-Wen Fu,*[b] and Xiao-Qing Yang*[a]

[a] *Brookhaven National Laboratory, Upton, NY 11973, USA*

[b] *Department of Chemistry, Fudan University, Shanghai, 200433, P.R.China*

[c] *Institute of Physics, Chinese academy of Sciences, Beijing, 100190, P.R. China*

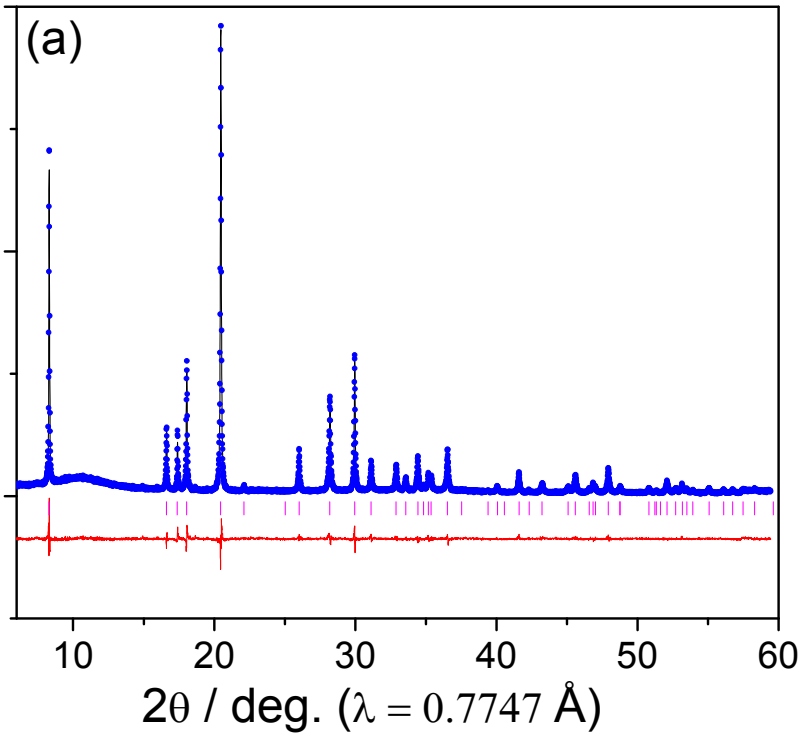

Fig. S1 Synchrotron diffraction pattern of $NaCrO_2$ and Rietveld refinement of its structure. The experimental (blue circles) and the calculated (black line) X-ray diffraction patterns are in good agreement with the smooth difference line (red line). The space group is R-3m. The calculated lattice parameters are: a=b=2.9768(6) Å, c= 16.9895(3) Å.

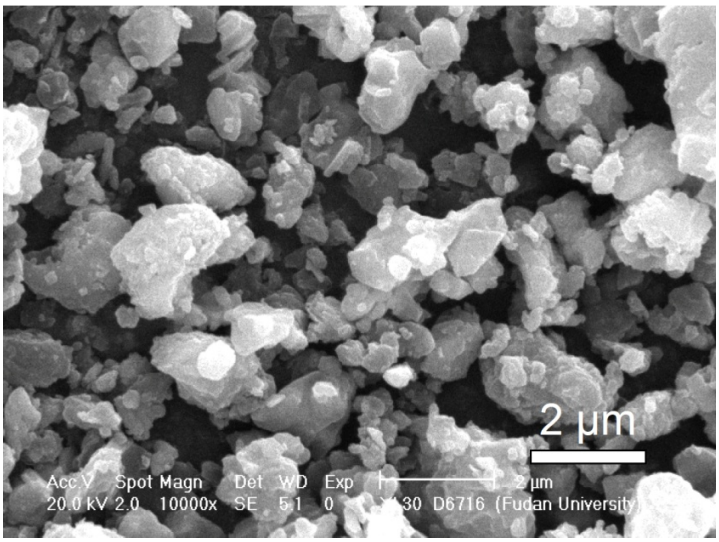

Fig. S2 SEM image of the pristine $NaCrO_2$ powder.

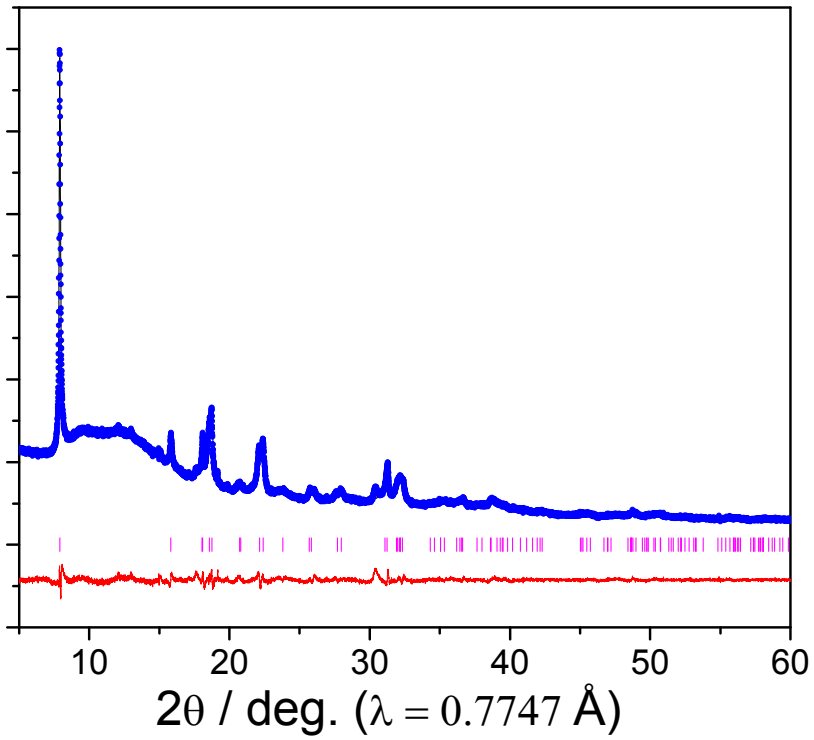

Fig. S3 *Ex-situ* synchrotron x-ray diffraction pattern of the fully charged $NaCrO_2$ ($\sim Na_{0.5}CrO_2$) and Rietveld refinement of its structure. The experimental (blue circles) and the calculated (black line) X-ray diffraction patterns are in good agreement with the smooth difference line (red line). It was indexed with a monoclinic cell (space group: C2/m) with the following parameters: a_M ($\sim\sqrt{3}\,a_R$) = 5.0178(7) Å, b_M ($\sim b_R$) = 2.8828(3), c_M ($\sim c_R/3\sin\beta$) = 5.9027(5) Å, β = 106.97°.

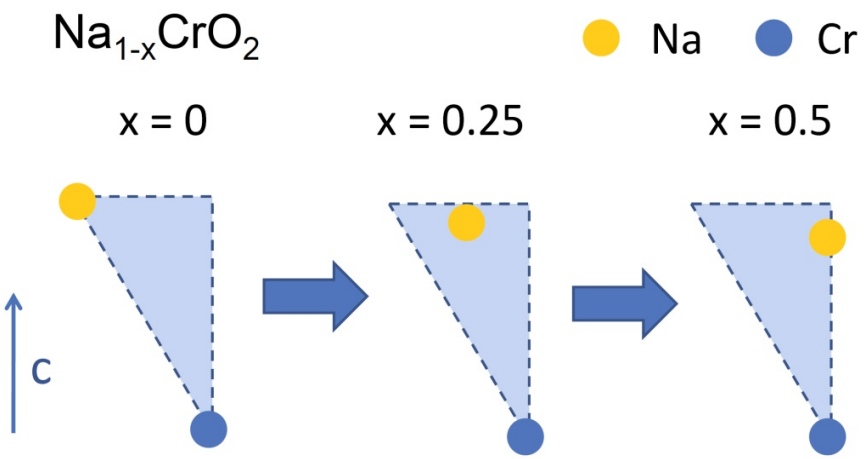

Fig. S4 Schematic for the relative position between Cr and Na ions in $Na_{1-x}CrO_2$ at different charge state (x=0, 0.25, 0.5). It corresponds to the Na coordination evolution from octahedral to pseudo-tetrahedral, then to trigonal-prismatic.