Electronic Supplementary Information for

Cation ordering in A-site-deficient Li-ion conducting perovskites La$_{(1-x)/3}$Li$_x$NbO$_3$

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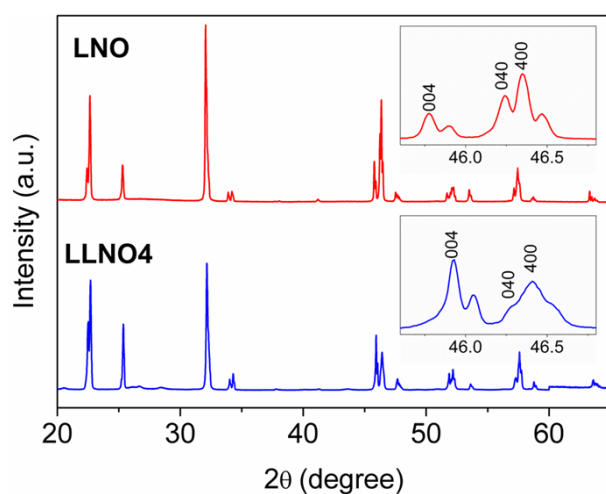

Fig. S1 Powder XRD patterns obtained from single-crystalline LNO and LLNO4 samples. Splitting of the (200) peaks shown in the insets indicates an orthorhombic crystal symmetry (space group C*mmm*) for both compounds. Calculation revealed their lattice parameters of LNO (a = 7.8129 Å, b = 7.8437 Å, c = 7.9364 Å) and LLNO4 (a = 7.7888 Å, b = 7.8252 Å, c = 7.9164 Å).
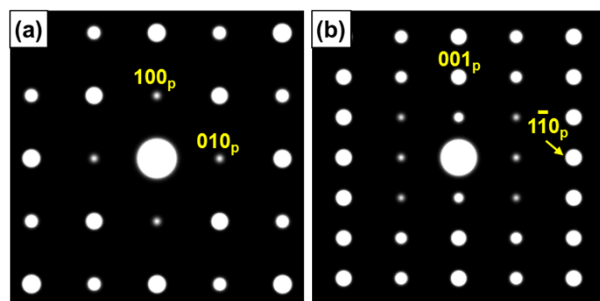

Fig. S2 Simulated (a) [001]$_p$ and (b) [110]$_p$ SAED patterns from the average crystal structure model of La$_{0.32}$Li$_{0.06}$NbO$_3$ (x = 0.06)[6] which has the same crystal symmetry (orthorhombic) and a similar Li content compared to LLNO4 (x = 0.04).
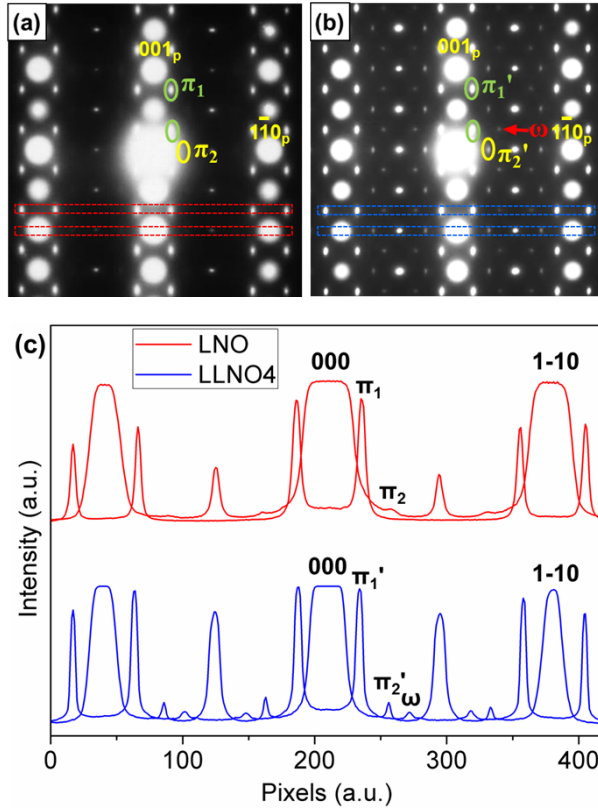
Fig. S3 SAED patterns taken from (a) LNO and (b) LLNO4 along their $[110]_p$ zone axes. (c) Intensity-scan profiles taken from the marked regions in (a) and (b) to reveal the positions of weak reflections, i.e. (π_1, π_2) of LNO and $(\pi_1', \pi_2'$ and $\omega)$ of LLNO4, along the $[1\text{-}10]_p$ direction.
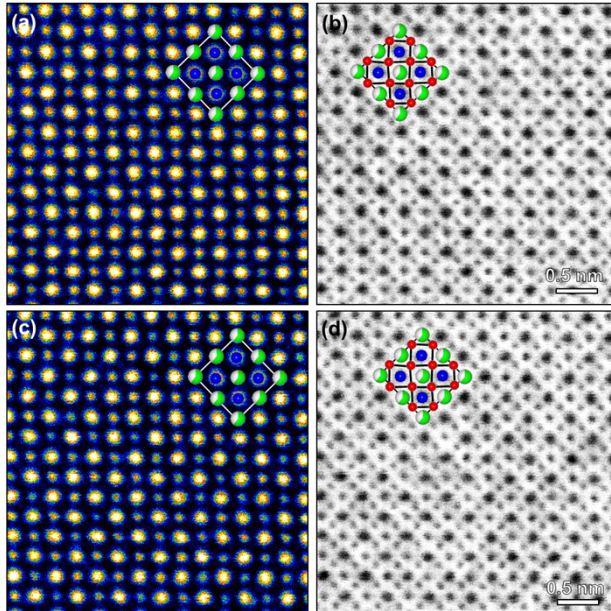

Fig. S4 $[001]_p$ zone-axis HAADF/ABF imaging. (a) HAADF and (b) ABF micrographs of LNO. (c) HAADF and (d) ABF micrographs of LLNO4. Overlaid structure models indicate the positions of O (red), Nb+O (blue) and La+vacancy (green) columns.