

Supporting information

Atomic and local electronic structures of $\text{Ca}_2\text{AlMnO}_{5+\delta}$ as an oxygen storage material

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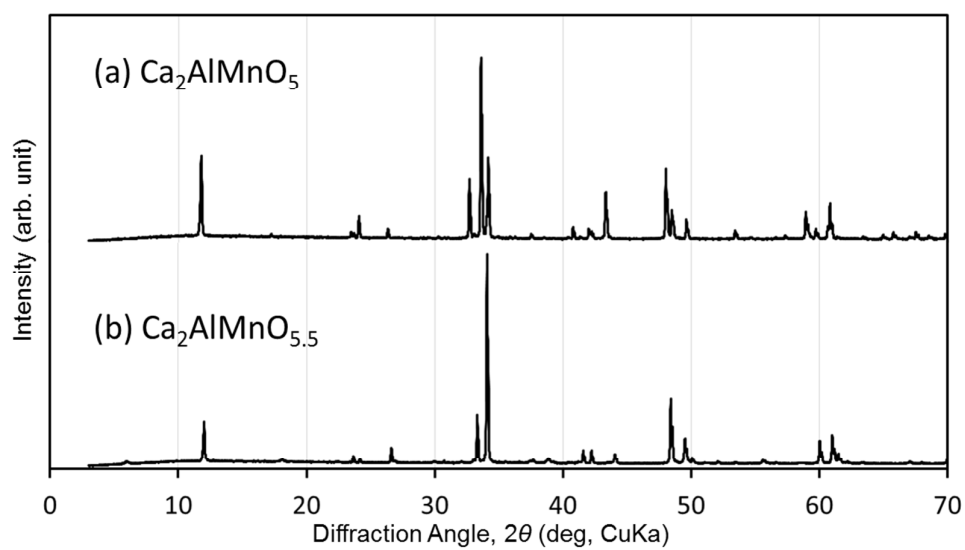


Fig. S1. XRD patterns of the synthesized powders.

Table S1. Structural parameters from Rietveld refinement.

	Ca ₂ AlMnO ₅	Ca ₂ AlMnO _{5.5}
	<i>I 2 m b</i>	<i>I m m a</i>
<i>a</i> , Å	5.24256(11)	5.25478(15)
<i>b</i> , Å	15.0051(3)	29.4266(9)
<i>c</i> , Å	5.47213(11)	5.37314(15)
<i>V</i> , Å ³	430.46(58)	830.85(05)
<i>R</i> <i>wp</i> , %	4.94	5.45
<i>R</i> <i>p</i> , %	3.73	4.07
<i>R</i> <i>e</i> , %	4.70	4.46
<i>S</i>	1.0508	1.2229
χ^2	1.1043	1.4954

Table S2. Atomic parameters for Ca₂AlMnO₅ and CaAlMnO_{5.5}.

Ca ₂ AlMnO ₅ (<i>I m a 2</i>)					
Atom	Occupancy	x	y	z	U _{iso} , Å ²
Ca	1.0	0.1121	0.5266	0.0072	0.00200
Mn	1.0	0	0	0	0.00550
Al	1.0	0.25	0.0726	0.0396	0.00520
O1	1.0	0.0115	0.2450	0.2440	0.00740
O2	1.0	0.1485	0.5660	0.4812	0.00400
O3	1.0	0.25	0.1427	0.3801	0.00500
Ca ₂ AlMnO _{5.5} (<i>I m m a</i>)					
Atom	Occupancy	x	y	z	
Ca1	1.0	0	0.0604	0.5106	
Ca2	1.0	0	0.1826	0.5259	
Mn	1.0	0	0.1254	0.0075	
Al1	0.5	0.0100	0.25	0.0440	
Al2	1.0	0	0	0	
O1	0.5	0.1220	0.25	0.3680	
O2	1.0	0	0.0695	0.0611	
O3	1.0	0	0.6993	0.0270	
O4	1.0	0.25	0.1392	0.25	
O5	1.0	0.25	0.5031	0.25	
O6	1.0	0.25	0.6259	0.25	

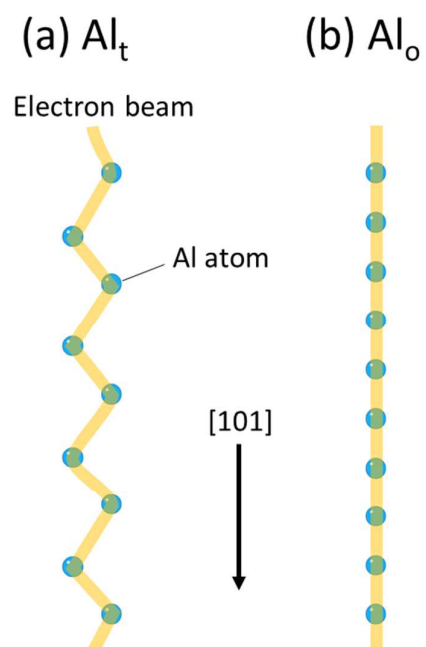


Fig. S2. Scheme of electron beam channeling at Al_t (tetrahedral) and Al_o (octahedral) sites.

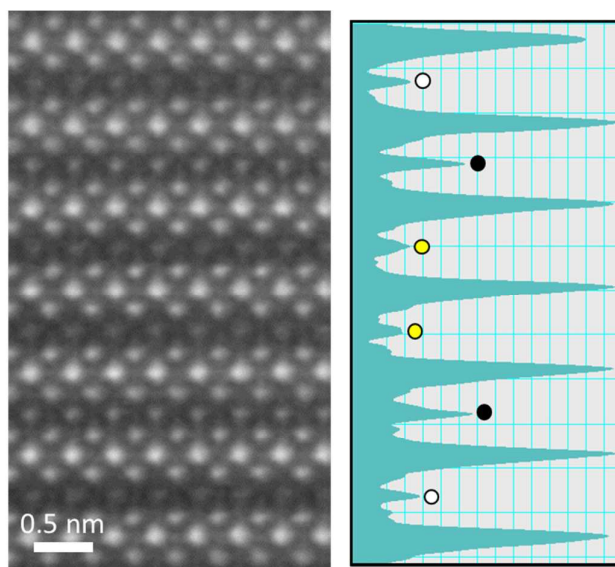


Fig. S3. Observed planar fault in $\text{Ca}_2\text{AlMnO}_{5.5}$, wherein two Al_t planes continuously arranged as a stacking error.

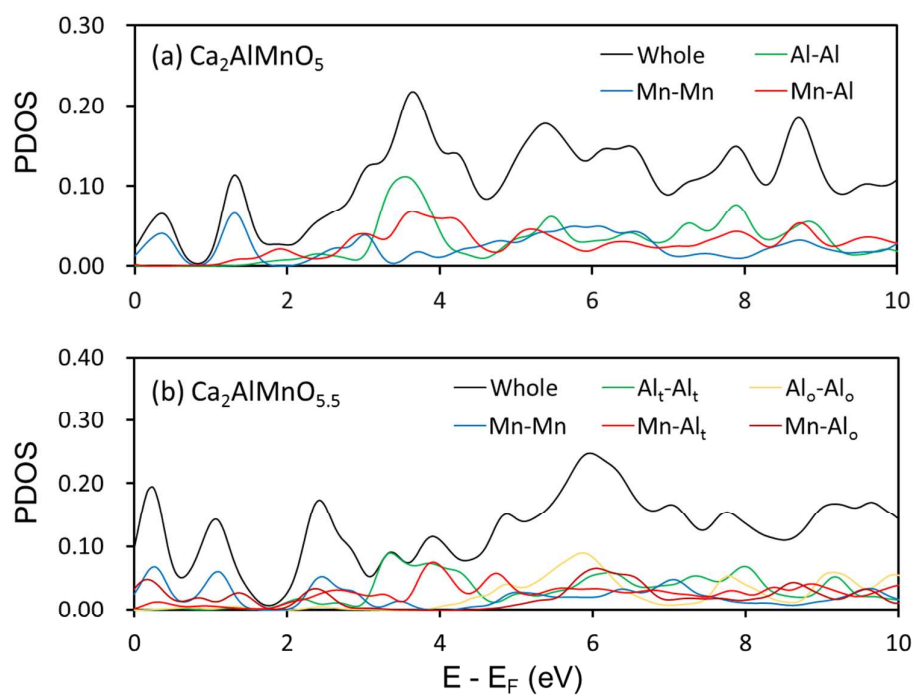


Fig. S4. Calculated O K-edge ELNES at each oxygen site in (a) $\text{Ca}_2\text{AlMnO}_5$ and (b) $\text{Ca}_2\text{AlMnO}_{5.5}$.