Supplementary Information

Oxide-ion diffusion in brownmillerite-type $Ca_2AlMnO_{5+\delta}$ from first-principles calculations

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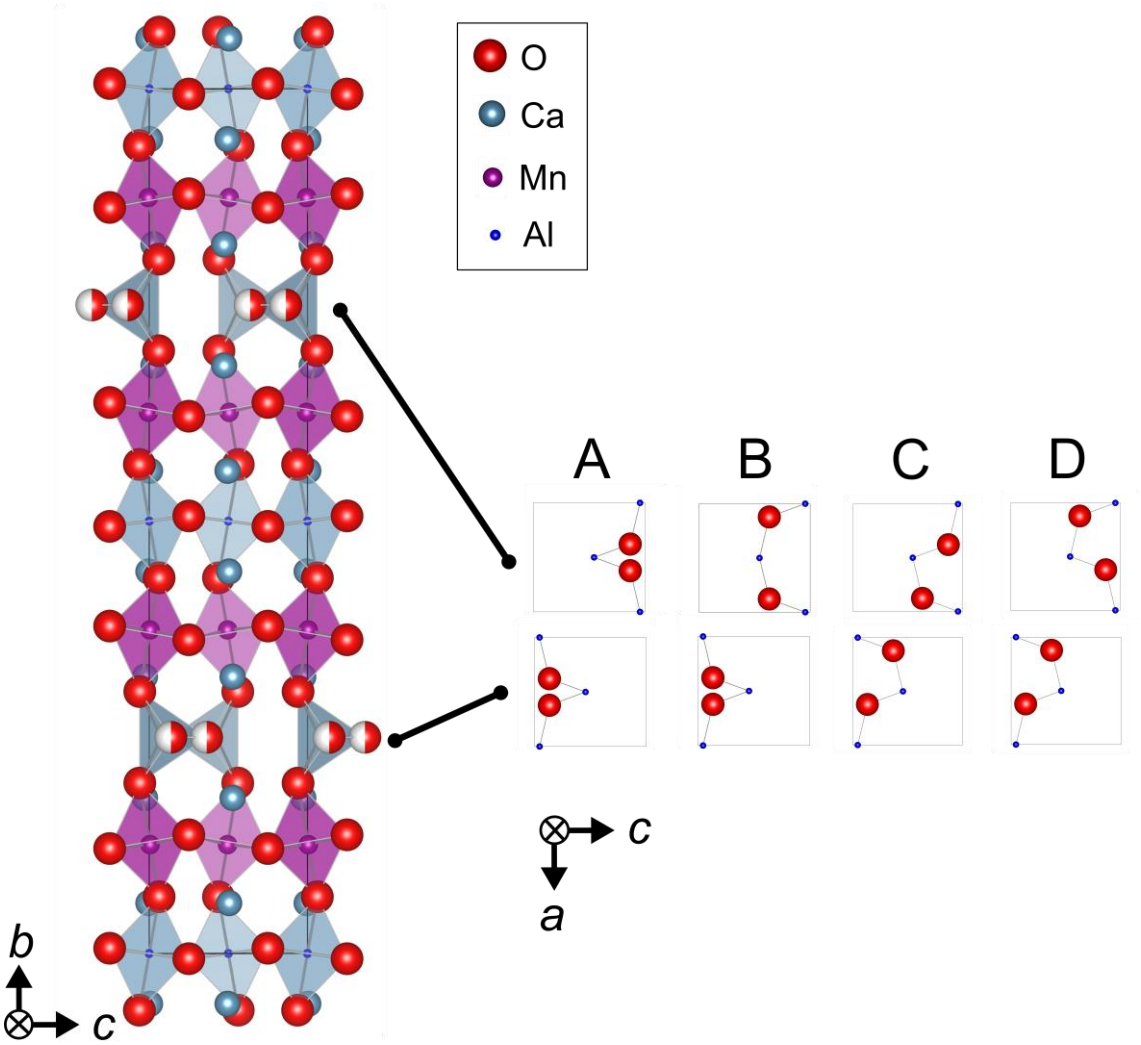

Figure S1 Four possible configurations (A-D) of Al and O atoms in AlO_4 layers of $Ca_2AlMnO_{5.5}$ corresponding to partial occupancies of 1/2. Grey lines indicate the unit cell.

Table S1 Relative energies, ΔE, of four AlO_4 layer configurations in $Ca_2AlMnO_{5.5}$ with respect to configuration D.

Config.	ΔE (eV/f.u.)
A	0.2824
B	0.2820
C	0.0002
D	0.0000

Table S2 Positional parameters and site occupancies in unit cells of Ca_2AlMnO_5 (space group *Ibm2*, $a = 5.501$ Å, $b = 14.79$ Å, $c = 5.250$ Å).

Atom	Wyckoff symbol	Fractional atomic coordinates			Site occupancy
		x	*y*	*z*	
Ca1	8*c*	0.5278	0.1115	0.0099	1.0
Mn1	4*a*	0.0000	0.0000	-0.0001	1.0
Al1	4*b*	0.0709	0.2500	0.0395	1.0
O1	8*c*	0.2462	0.0143	0.2519	1.0
O2	8*c*	0.9283	0.1476	0.9676	1.0
O3	4*b*	0.3596	0.2500	0.8767	1.0
X	4*b*	0.6721	0.2500	0.1693	
Y	4*b*	0.9153	0.7500	0.7057	

Table S3 Positional parameters and site occupancies in unit cells of $Ca_2AlMnO_{5.5}$ (space group *Imma*, $a = 5.280$ Å, $b = 29.12$ Å, $c = 5.390$ Å).

Atom	Wyckoff symbol	Fractional atomic coordinates			Site occupancy
		x	*y*	*z*	
Ca1	8*h*	0.9971	0.0582	0.5055	1.0
Ca2	8*h*	0.0051	0.3206	0.5305	1.0
Mn1	8*h*	0.9976	0.1260	0.0083	1.0
Al1	4*a*	0.9972	0.0000	0.0000	1.0
Al2	8*i*	0.0495	0.2500	0.0769	0.5
O1	8*g*	0.2474	0.9931	0.2499	1.0
O2	8*g*	0.2491	0.1394	0.2469	1.0
O3	8*g*	0.2496	0.6206	0.2475	1.0
O4	8*h*	0.9963	0.0656	0.0703	1.0
O5	8*h*	0.9892	0.3031	0.9372	1.0
O6	8*i*	0.8862	0.2500	0.3668	0.5