Supporting Information For

Quantum Chemical Design of Doped $Ca_2MnAlO_{5+\delta}$ as Oxygen Storage Media

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Table S1. Cartesian coordinates of Ca_2MnAlO_5 relaxed by density functional theory (*a*=5.601 Å; *b*=15.007 Å; *c*=5.337 Å)

	x	y	z
Ca	0.180126	1.69171	2.621628
Ca	5.421301	13.31568	2.621628
Ca	5.421301	9.195407	2.621628
Ca	0.180126	5.811987	2.621628
Ca	2.980839	9.195407	5.290126
Ca	2.620588	5.811987	5.290126
Ca	2.620588	1.69171	5.290126
Ca	2.980839	13.31568	5.290126
Mn	0	0	0.010944
Mn	0	7.503697	0.010944
Mn	2.800714	7.503697	2.679442
Mn	2.800714	0	2.679442
Al	5.186821	3.751849	5.132896
Al	0.414607	11.25555	5.132896
Al	2.386107	11.25555	2.464398
Al	3.21532	3.751849	2.464398
O	1.417849	14.80928	1.337153
O	4.183578	0.198112	1.337153
O	4.183578	7.305585	1.337153
O	1.417849	7.701809	1.337153
O	4.218562	7.305585	4.005651
O	1.382865	7.701809	4.005651
O	1.382865	14.80928	4.005651
O	4.218562	0.198112	4.005651
O	0.391226	2.234028	0.172142
O	5.210201	12.77337	0.172142
O	5.210201	9.737725	0.172142
O	0.391226	5.269669	0.172142
O	3.19194	9.737725	2.840641
O	2.409487	5.269669	2.840641
O	2.409487	2.234028	2.840641
O	3.19194	12.77337	2.840641
O	4.798276	3.751849	3.351951
O	0.803151	11.25555	3.351951
O	1.997562	11.25555	0.683453
O	3.603865	3.751849	0.683453

Table S2. Cartesian coordinates of $Ca_2MnAlO_{5.5}$ relaxed by density functional theory (*a*=5.291 Å; *b*=29.696 Å; *c*=5.451 Å)

	x	y	z
Ca	-0.000012	1.671190	2.726163
Ca	-0.000012	28.024639	2.725326
Ca	-0.000012	13.176725	2.726163
Ca	-0.000012	16.519105	2.725326
Ca	2.645689	16.519105	0.000419
Ca	2.645689	13.176725	-0.000419
Ca	2.645689	28.024639	0.000419
Ca	2.645689	1.671190	-0.000419
Ca	0.042239	9.527329	2.886652
Ca	0.042239	20.168501	2.564838
Ca	0.042239	5.320586	2.886652
Ca	0.042239	24.375243	2.564838
Ca	2.687940	24.375243	0.160907
Ca	2.687940	5.320586	5.290583
Ca	2.687940	20.168501	0.160907
Ca	2.687940	9.527329	5.290583
Mn	0.000251	3.713380	0.043704
Mn	0.000251	25.982450	5.407785
Mn	0.000251	11.134535	0.043704
Mn	0.000251	18.561294	5.407785
Mn	2.645952	18.561294	2.769449
Mn	2.645952	11.134535	2.682040
Mn	2.645952	25.982450	2.769449
Mn	2.645952	3.713380	2.682040
Al	-0.000737	0.000000	0.000000
Al	-0.000737	14.847915	0.000000
Al	2.644964	14.847915	2.725745
Al	2.644964	0.000000	2.725745
Al	0.284626	7.423957	0.421422
Al	0.284626	22.271872	5.030068
Al	2.930327	22.271872	3.147167
Al	2.930327	7.423957	2.304323
O	1.322169	29.514727	1.362142
O	3.967870	0.181102	4.087887
O	3.967870	15.029017	1.363603
O	1.322169	14.666812	4.089348
O	3.967870	14.666812	4.087887
O	1.322169	15.029017	1.362142
O	1.322169	0.181102	4.089348
O	3.967870	29.514727	1.363603
O	1.335923	4.117267	1.344836
O	3.981624	25.578561	4.070581

O	3.981624	10.730648	1.380908
O	1.335923	18.965182	4.106653
O	3.981624	18.965182	4.070581
O	1.335923	10.730648	1.344836
O	1.335923	25.578561	4.106653
O	3.981624	4.117267	1.380908
O	1.329553	18.414089	1.356365
O	3.975254	11.281741	4.082109
O	3.975254	26.129655	1.369380
O	1.329553	3.566174	4.095125
O	3.975254	3.566174	4.082109
O	1.329553	26.129655	1.356365
O	1.329553	11.281741	4.095125
O	3.975254	18.414089	1.369380
O	-0.005746	1.925173	0.374832
O	-0.005746	27.770655	5.076658
O	-0.005746	12.922741	0.374832
O	-0.005746	16.773089	5.076658
O	2.639955	16.773089	3.100576
O	2.639955	12.922741	2.350913
O	2.639955	27.770655	3.100576
O	2.639955	1.925173	2.350913
O	-0.073538	8.987369	5.115971
O	-0.073538	20.708462	0.335519
O	-0.073538	5.860546	5.115971
O	-0.073538	23.835282	0.335519
O	2.572163	23.835282	2.390226
O	2.572163	5.860546	3.061263
O	2.572163	20.708462	2.390226
O	2.572163	8.987369	3.061263
O	4.709051	22.271872	3.459809
O	4.709051	7.423957	1.991680
O	2.063350	7.423957	0.734065
O	2.063350	22.271872	4.717425

Table S3. Lattice parameters of Sr_2MnAlO_5 calculated by density functional theory using different structure models.

Ca_2MnAlO_5 model			
a (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
5.756	16.011	5.462	503.4
Sr_2MnAlO_5 model			
a (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
5.526	15.499	5.619	481.3
experiment			
a (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
5.436	15.623	5.608	476.2