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Electronic Supplementary Information (ESI)

First-principles computational studies on layered $Na_2Mn_3O_7$ as a high-rate cathode material for sodium ion batteries

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Table S1 The energy change (in eV) caused by each Na removal at every deintercalation stage. The most energetically favored configurations for each deintercalation stage are shown in bold.

x in $Na_xMn_3O_7$	Na1	Na2	Na3	Na4
2	+2.341	**+2.081**	+2.082	+2.341
1.5	+2.365		**+2.171**	+2.390
1	+2.536			**+2.534**
0.5	**+2.803**			

Table S2 The energy change (in eV) caused by each Na addition at every intercalation stage.

x in $Na_xMn_3O_7$	Na2	Na3	Na4
1	–2.075	–2.075	
0.5	–2.342	–2.314	–2.534

Table S3 Lattice parameters (Å) and cell volume (Å^3) at every deintercalation stage. The lattice used in calculation are $Na_{2x}Mn_6O_{14}$ originated from that in Figure 1. V_{change} shows the volume change of the corresponding structure compared with the original $Na_4Mn_6O_{14}$ cell.

x in $Na_xMn_3O_7$	a	b	c	volume	V_{change}(%)
2.0	7.68	7.66	6.77	283.32	-
1.5	7.65	7.61	6.88	279.95	-1.19
1.0	7.61	7.59	6.82	270.35	-4.58
0.5	7.62	7.61	6.80	269.58	-4.85
0	7.52	7.49	5.94	226.35	-20.11

Table S4 Average transferred Bader Charge (e) of O, Na and Mn at every deintercalation stage. The positive value and negative value represent the gaining and loss of electrons, respectively.

x in $Na_xMn_3O_7$	O	Na	Mn
2.0	1.04	-0.87	-1.85
1.5	0.98	-0.88	-1.86
1.0	0.92	-0.88	-1.86
0.5	0.86	-0.89	-1.86

Table S5 O-evolution energy (eV) of $Na_xMn_3O_7$.

x in $Na_xMn_3O_7$	0.5	1	1.5	2
E	0.13	0.40	0.58	0.94

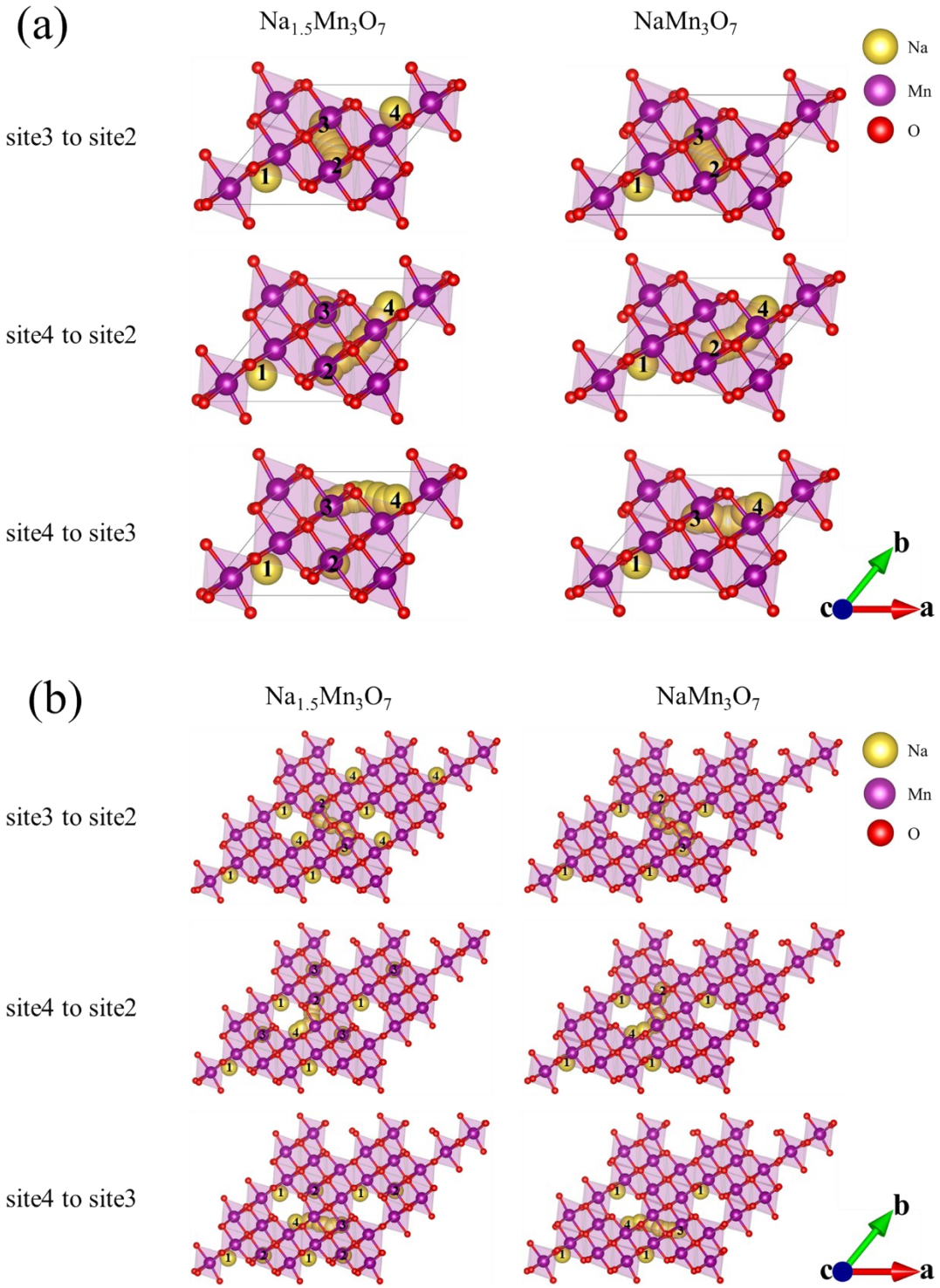

Fig. S1 Schematic representation of the optimized Na migration pathways (a) inside one single cell and (b) between adjacent cells. In (b), only one migrating Na among four cells is shown for clarity.