Support information

Figure S1 Comparison of the calculated energy barriers for Li-ion diffusion and Mn-ion migration in LiMnO$_2$ with two “semi-core” states for Mn.

Figure S2a Optimization of Li$_{0.5}$MnO$_2$ by the Ewald method.

Figure S2b The schematic structure of monoclinic Li$_{0.5}$MnO$_2$ (C2/m).
Figure S2c Comparison of the calculated energy barriers for Mn-ion migration into the Li- and Na-layers layer in $A_{0.5}\text{MnO}_2$ ($A=\text{Li, Na}$).