Support information

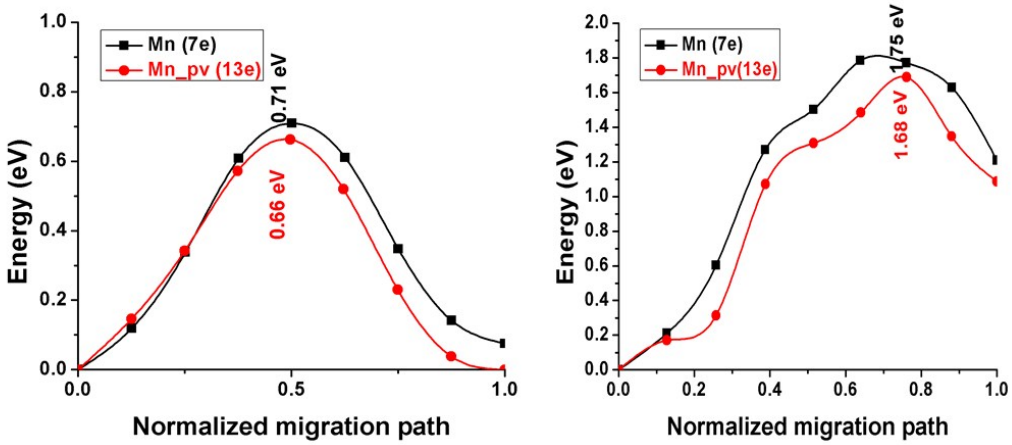

Figure S1 Comparison of the calculated energy barriers for Li-ion diffusion and Mn-ion migration in $LiMnO_2$ with two "semi-core" states for Mn.

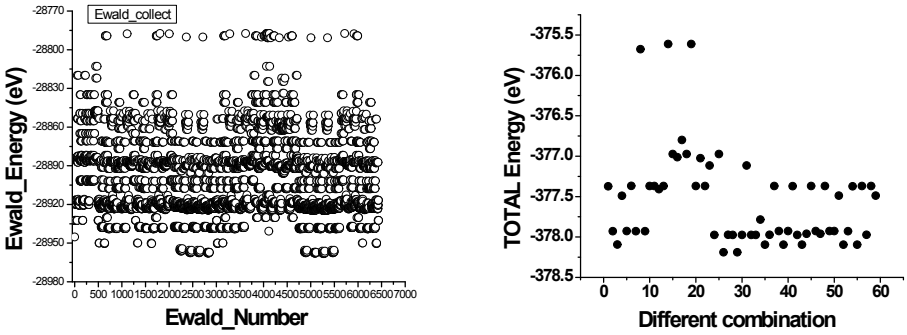

Figure S2a Optimization of $Li_{0.5}MnO_2$ by the Ewald method.

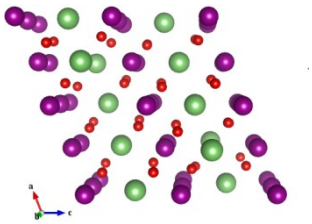

Figure S2b The schematic structure of monoclinic $Li_{0.5}MnO_2$ (C2/m).

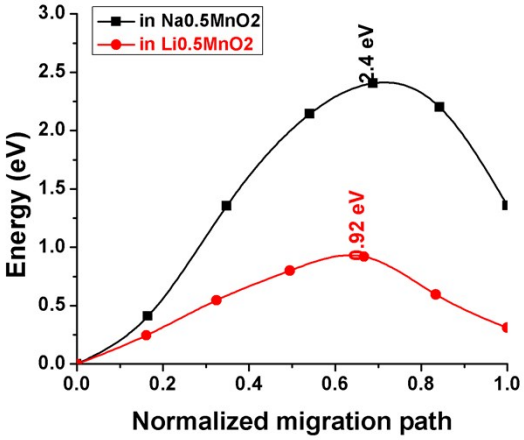

Figure S2c Comparison of the calculated energy barriers for Mn-ion migration into the Li- and Na-layers layer in $A_{0.5}MnO_2$ (A=Li, Na).