Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

β-MnO_2 as cathode material for lithium ion batteries from first principles calculations

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Table S1. Relative single-point energies of MnO_2-$LiMnO_2$ calculated from HSE[a]

	MnO_2	$Li_{0.5}MnO_2$	$Li_{0.75}MnO_2$	$Li_{0.875}MnO_2$	$LiMnO_2$
AFM	0	0	0	0	0
FM	37	44	-19	-18	-9

[a] The single-point energies of the AFM state are set as 0 meV.

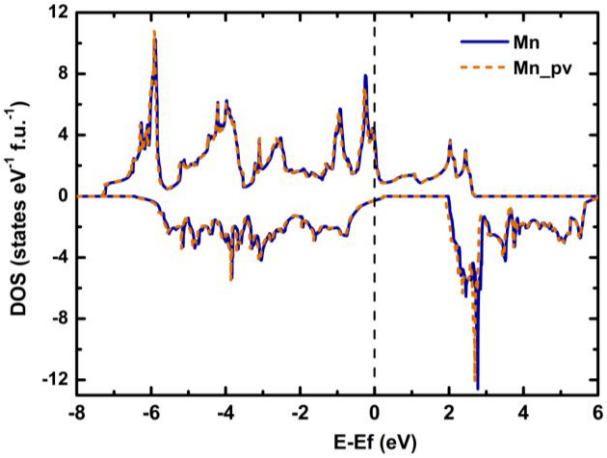

Figure S1. Total density of states of β-MnO_2 calculated by PBE+U. Valence electron configurations of the pseudopotential for Mn were taken as $3d^6$ $4s^1$ (royal solid line) and $3p^6 3d^6$ $4s^1$ (orange dash line) , respectively. The Fermi level is set to be 0.

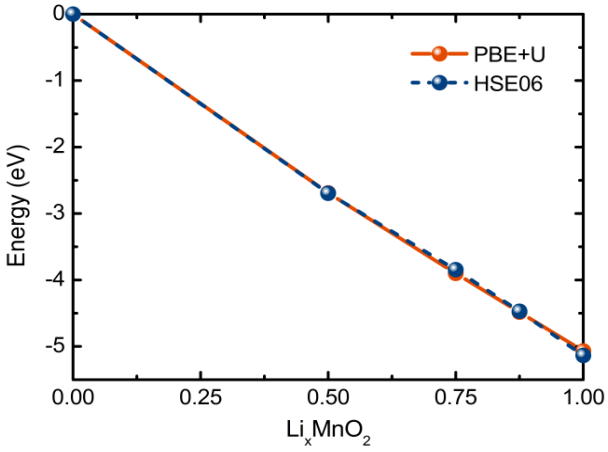

Figure S2. The relative energy values (ΔE) of Li_xMnO_2 calculated by PBE+U and HSE functional, respectively. The energy of MnO_2 is set to be 0.

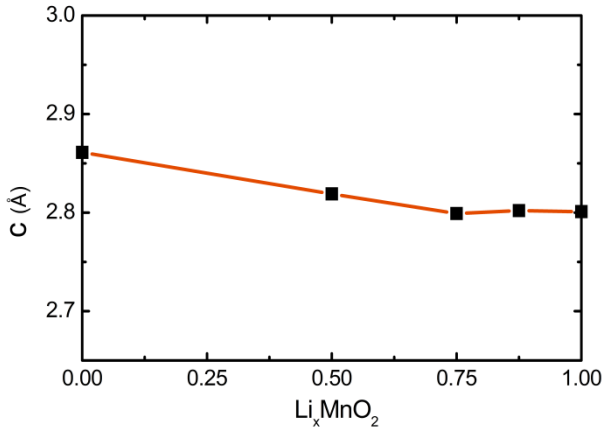

Figure S3. Lattice parameter c of Li_xMnO_2 calculated using HSE functional.

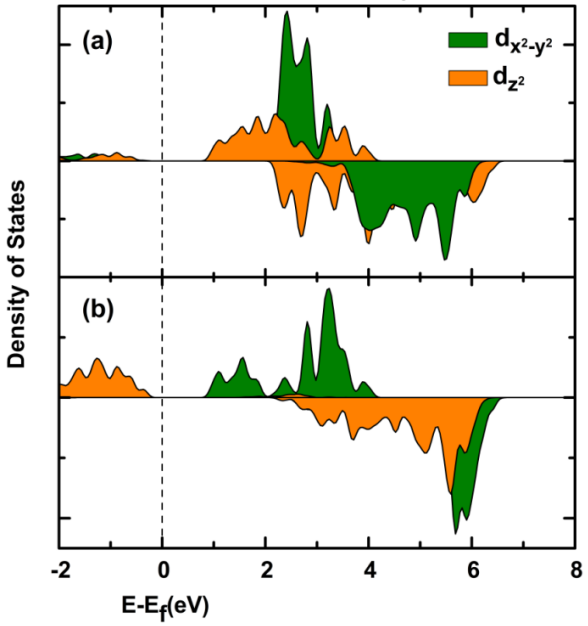

Figure S4. The Mn-3d projected density of states on (a) Mn_a and (b) Mn_b in $Li_{0.5}MnO_2$ calculated using HSE functional. The olive and orange filled area is denoted as $d_{x^2-y^2}$ and d_{z^2}, respectively. The Fermi level is set to be 0.