Supplementary Information

Influence of Magnetic Ordering and Jahn-Teller Distortion on the Lithiation Process of LiMn$_2$O$_4$

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Figure S1 Calculations of (a) energies and (b) lattice constants as a dependence of U-J=4.2, 4.5, 4.8, 5.1 eV for AFM-1, AFM-2 and FM configurations.
Figure S2 Energies of AFM and FM LMO structures in the cubic phase (cyan) and the orthorhombic phase (red).

Figure S3 Projected density of state of Mn-3d (a) and O-2p (b) states in AFM-I. The solid and dashed lines in the left panel represent Mn-$e_g$ and -$t_{2g}$ orbitals, respectively. The solid and dashed lines in the right panel represent O-$p_{xy}$ and -$p_z$ orbitals, respectively. Zero energy denotes the position of the Fermi level.