Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Influence of Magnetic Ordering and Jahn-Teller Distortion on the Lithiation Process of $LiMn_2O_4$

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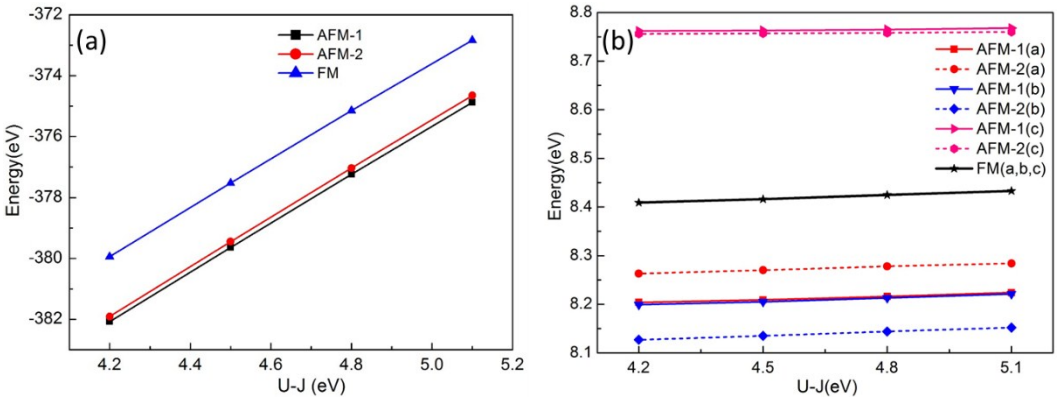

Figure S1 Calculations of (a) energies and (b) lattice constants as a dependence of U-J=4.2, 4.5, 4.8, 5.1 eV for AFM-1, AFM-2 and FM configurations.

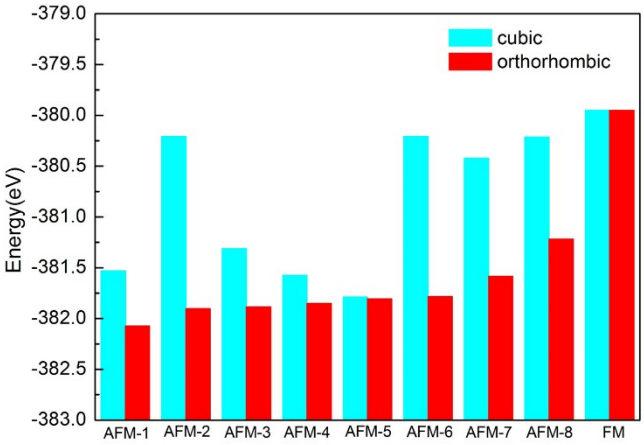

Figure S2 *Energies of AFM and FM LMO structures in the cubic phase (cyan) and the orthorhombic phase (red).*

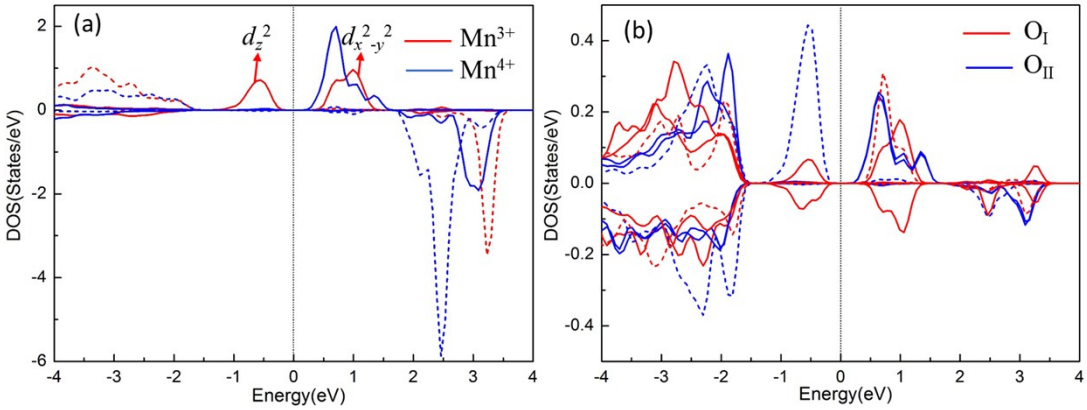

Figure S3 *Projected density of state of Mn-3d (a) and O-2p (b) states in AFM-1. The solid and dashed lines in the left panel represent Mn-e_g and -t_{2g} orbitals, respectively. The solid and dashed lines in the right panel represent O-$p_{x,y}$ and -p_z orbitals, respectively. Zero energy denotes the position of the Fermi level.*