Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Influence of Valance and Magnetism on the Jahn-Teller Distortion in LiMn2O4 and its Lithiation Process[1] WEIWEI LIU, Beijing Computational Science Research Center, YANNING ZHANG, Univ of Electronic Sci Tech — We performed extensive first-principles studies on the valence and magnetic configurations of spinel $LiMn_2O_4$, a promising candidate of cathode materials in Li-ion batteries. We find that the ground state of $LiMn_2O_4$ is an anti-ferromagnetic (AFM) orthorhombic spinel structure, where AFM Mn^{3+} layer and FM Mn^{4+} layer alternate along the [001] direction and the 90Mn^{3+}-O^{2-}-Mn^{3+} in Mn^{3+}-(001) planes is in AFM coupling, forming the indirect Kramers-Anderson superexchange. The coplanar Jahn-Teller (JT) ions maximize the JT distortion and the AFM magnetic orderings further strengthen the interaction between Mn^{3+} cations and O^{2-} anions, making the structure stable. Li diffusion in such a stable $LiMn_2O_4$ will go through a ring consisting of six Mn atoms, and the energy barrier of Li diffusion is dependent on the valence states of Mn atoms. Our theoretical results give insights in exploring ground state of related JT magnetic materials, and also provide information for the performance improvement of $LiMn_2O_4$ cathode materials.

[1]Work was supported by the startup fund of China Thousand Young Talents, National Basic Research Program of China (973 program, No. 2013CB934700). The calculations were supported by Tianhe2-JK in Beijing Computational Science Research Center.

Yanning Zhang
Univ of Electronic Sci
Tech

Date submitted: 09 Nov 2016 Electronic form version 1.4