Abstract Submitted for the MAR08 Meeting of The American Physical Society

Structural and physical properties of Fe-doped LiMn<sub>2</sub>O<sub>4</sub> oxides<sup>1</sup> YANG LI, Department of Engineering Science and Materials, University of Puerto Rico at Mayaguez, PR 00681, USA, BOYU MA, NING CHEN, YANG LIU, WEIPENG WANG, AIHUA WANG, XINGQIAO MA, GUOHUI CAO, Department of Physics, University of Science and Technology Beijing, 100083, China — A joint experimental and theoretical study of the physical property and electronic structures in Fe-doped LiMn<sub>2</sub>O<sub>4</sub> has been performed. The samples with pure phase are prepared by the solid reaction. The X-ray diffraction refinement and SEM analysis show that Fe enters lattice to occupy Mn site. The physical property measurements indicate that Fe doping results in modification of microstructure. The physical properties heavily depend on Fe-doping concentration. The first-principles simulations show that charge ordering and magnetic ordering occur in Fe-doped samples. The d electron increasing in the system results in carrier concentration changing.

<sup>1</sup>This work was supported in part by National Natural Science Foundation of Beijing (Grant No. 1072007), and National Science Foundation PREM program (Grant No. 0351449)

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Date submitted: 28 Dec 2007

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