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

Supporting Information for

Tuning polaronic redox behavior in Olivine phosphate

Yue Gu, Mouyi Weng, Gaofeng Teng, Hua Zeng, Jianshu Jie, Weiji Xiao, Jiaxin Zheng*, and Feng Pan*

School of Advanced Materials, Peking University, Shenzhen Graduate School, Shenzhen 518055, People's Republic of China

*Corresponding authors: J. Z. (zhengjx@pkusz.edu.cn) and F. P. (panfeng@pkusz.edu.cn)

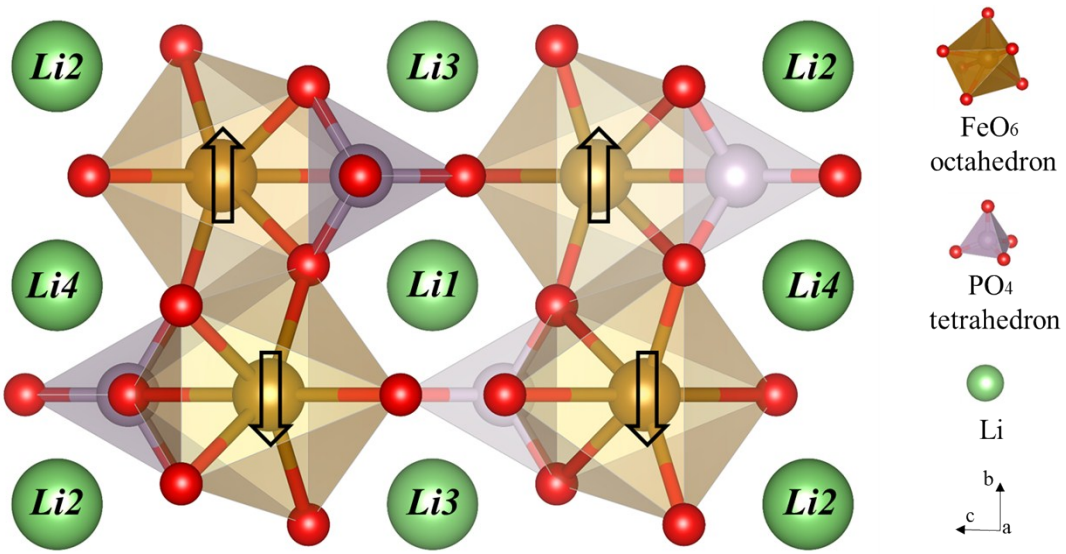

Fig. S1 The direction of the magnetic moment of each Fe ion in the $LiFePO_4$ cell.

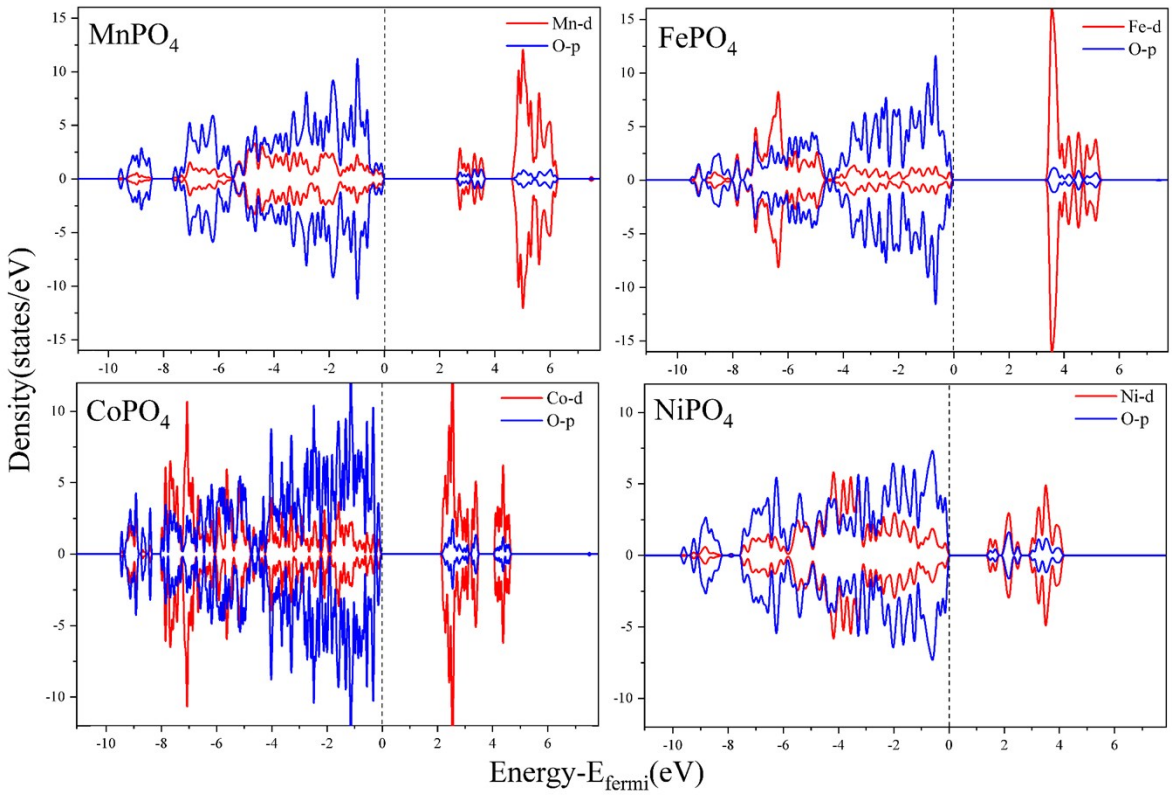

Fig. S2 The HSE06 calculated partial density of states of MPO_4 (M = Mn, Fe, Co, Ni).

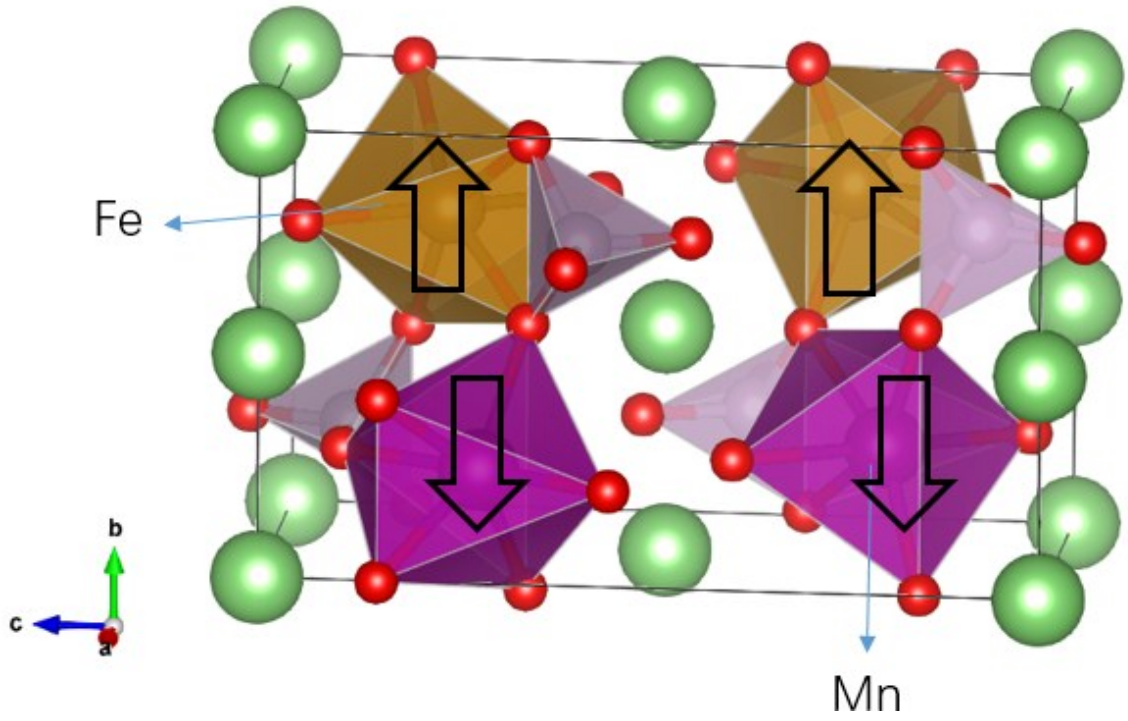

Fig. S3 The $LiFe_{0.5}Mn_{0.5}PO_4$ cell which has the lowest energy (antiferromagnetic conditions).

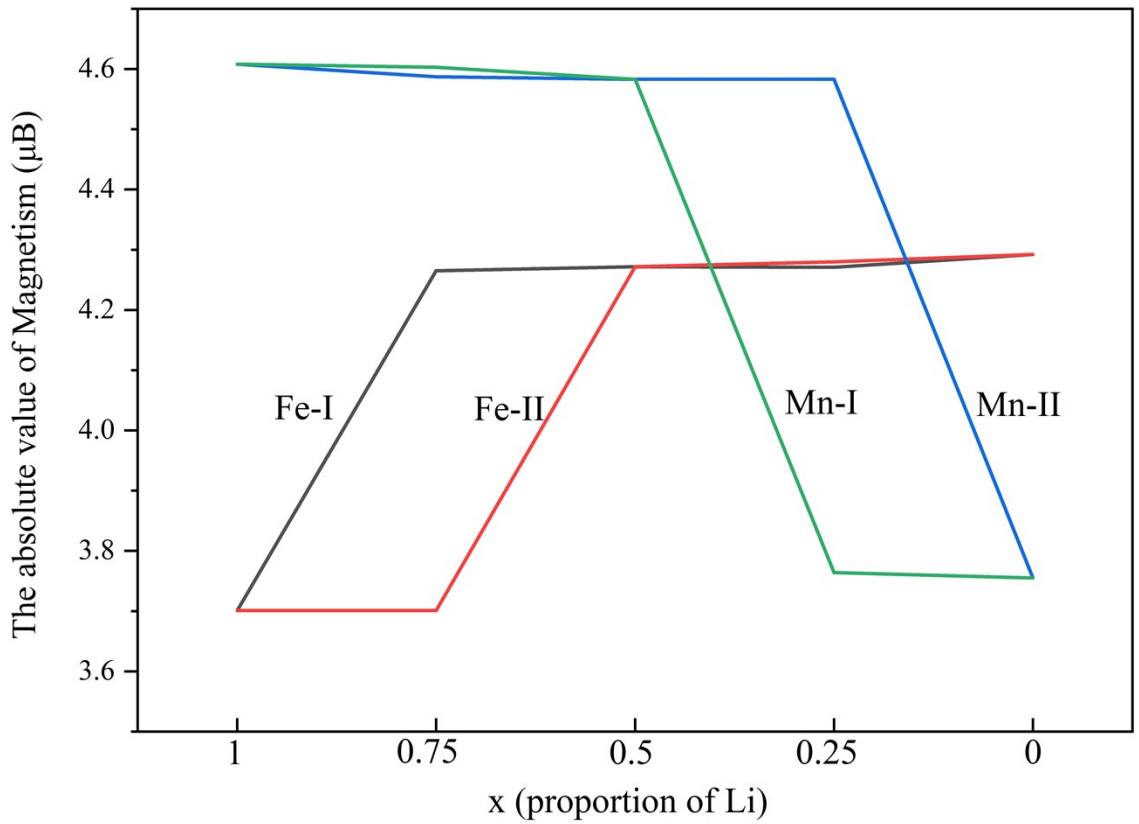

Fig. S4 The absolute value of calculated magnetic moments of four transition metal ions in $Li_xFe_{0.5}Mn_{0.5}PO_4$ (x = 1, 0.75, 0.5, 0.25, 0).

Tab. S1 The calculated magnetic moments of four Fe ions in Na_xFePO_4 (x = 1, 0.75, 0)

	Fe-I	**Fe-II**	**Fe-III**	**Fe-IV**
$NaFePO_4$	3.702	-3.702	3.702	-3.702
$Na_{0.75}FePO_4$	3.706	-3.707	3.690	-4.262
$FePO_4$	4.283	-4.283	4.283	-4.283