Supporting Information:

Systematic study on carrier transport processes in charging olivine phosphates LiMPO$_4$ (M = Fe,Mn) by hybrid DFT calculations

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Table S1: Ratio of the magnetic moments on the two TM sites between which a h^+ hops. Each figure denotes the value for the initial/final TM site (denoted as s1 and s2) on which the h^+ localizes in the hopping process. These values were obtained by dividing the magnetic moment on each TM site at the transition state with that at the initial state of the h^+ hopping process. The magnetic moments were obtained by DFT calculations using the HSE06 functional with the fraction of Hartree-Fock exchange (HFX) modified, which ranges from 25% to 50%.

HFXx%	site	25	30	35	40	45	50
LFP	s1	0.965	0.979	0.993	1.00	1.00	1.00
	s2	1.06	1.03	1.01	1.00	1.00	1.00
LMP	s1	1.13	1.10	1.12	1.09	1.05	1.04
	s2	0.937	0.935	0.938	0.963	0.991	0.994

For example, the magnetic moments on s1 and s2 calculated by using the HSE06 functional with 25% fraction of HFX are 4.26 and 3.71, respectively, at the initial state of the hopping process in LFP. Since the corresponding values at the transition state are 4.11 and 3.92, the ratios on s1 and s2 sites become $4.11/4.26 = 0.965$ and $3.92/3.71 = 1.06$, respectively. If the h^+ remains localized almost completely on s1 even at the transition state, the magnetic moments on s1 and s2 hardly change during the hopping process and the ratios of those at the transition state to those at the initial state become almost 1.

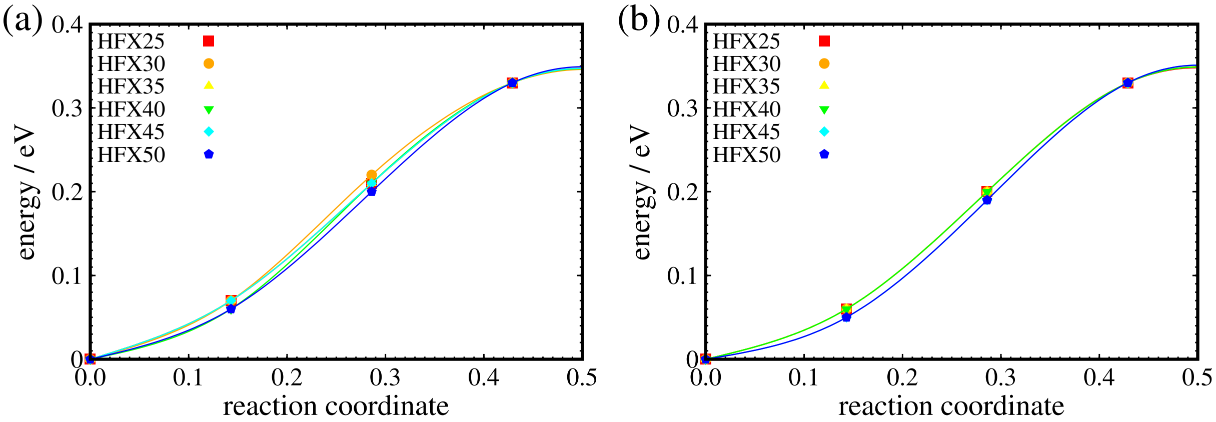

Figure S1: Energy profiles of free V_{Li} hopping whose path was determined by a nudged elastic band calculation for (a) LFP and (b) LMP. The reaction coordinate corresponds to the relative distance of each image from the initial image, scaled by that of the final image. The plots show the results of DFT calculations with the HSE06 functional with the fraction of Hartree-Fock exchange (HFX) increased from the original value of 25% to 50% by 5%.