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Molecular Dynamics Simulations on Lithium Diffusion in $LiFePO_4$: the effect of anti-site defects

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I. Structure information

The parameters for the initial and fully relaxed structures of $LiFePO_4$ are given in Table S1 and S2, respectively.

Table S1 Structural parameters and fractional coordinates of $LiFePO_4$ for calculations

LiFePO4: Space Group Pnma **a) 10.3377(5) Å, b) 6.0112(2) Å, c) 4.6950(2) Å**			
ion	**x**	**y**	**z**
Li	0.0000	0.0000	0.0000
Fe	0.2822(2)	0.2500	0.9738(5)
P	0.0950(3)	0.2500	0.418(6)
O(1)	0.09713(3)	0.2500	0.7428(7)
O(2)	0.4573(3)	0.2500	0.2067(7)
O(3)	0.166(3)	0.0464(4)	0.2851(4)

Table S2 Calculated and experimental structural parameters of $LiFePO_4$

(i) Unit Cell Parameters

parameter	**calculated**	**Cal.1**[a]	**Cal.2**[b]	**Cal.3**[c]	**Exp.1**[d]	**Exp.2**[e]
a **(Å)**	10.41	10.41	10.44	10.45	10.43	10.34
b**(Å)**	6.08	6.08	6.05	6.05	6.10	6.01
c**(Å)**	4.79	4.81	4.74	4.74	4.74	4.70

(ii) Bond Lengths

ion pair	**Cal.**	**Cal.1**[f]	**Cal.2**[g]	**Exp.1**[f]	**Exp.2**[g]
Li-O	2.16 2.19 2.24	2.10 2.19 2.24	2.05 2.10 2.16	2.09 2.17 2.19	2.14 2.15 2.24
Fe-O	2.10 2.16 2.20 2.32	2.05 2.06 2.19 2.24	2.02 2.05 2.13 2.17	2.06 2.12 2.20 2.25	1.98 2.04 2.23 2.29
P-O	1.51 1.52 1.53	1.51 1.56 1.57	1.53 1.54 1.56	1.53 1.54 1.56	1.50 1.53 1.57

a) Ref1, b) Ref 2, c) Ref 3 , d) Ref 4, e) Ref 5, f) Ref 6, g) Ref 7.

II. Dynamical properties

a. MSD functions of Li ions in bulk $LiFePO_4$.

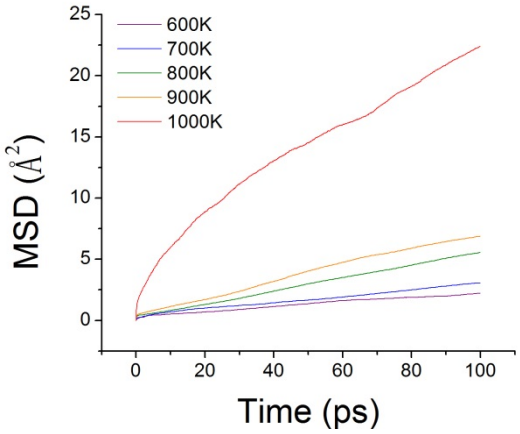

Figure S1 MSD of Li^+ along the [010] direction at T = 600, 700, 800, 900, 1000 K in $LiFePO_4$

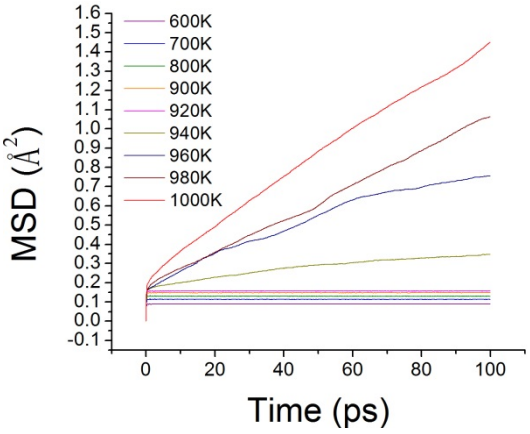

Figure S2 MSD of Li^+ along the [001] direction at T = 600, 700, 800, 900, 1000 K in $LiFePO_4$

b. Diffusion coefficients and activation energy of Li ions in pure $LiFePO_4$.

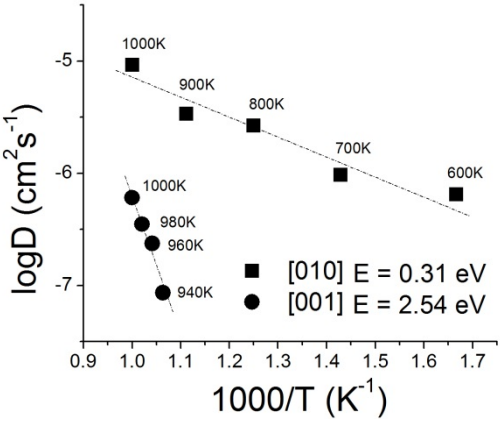

Figure S3 Diffusion coefficients and ctivation energies of Li^+ diffusion along the [010] and [001] directions in $LiFePO_4$

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