SUPPLEMENTARY INFORMATION FOR

High-throughput design and optimization of fast lithium ion conductors by the combination of bond-valence method and density functional theory

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Table S1. The activation energies (E_a) of lithium migration calculated by BV-based method and DFT method for 46 compounds.

No.	Compounds	E_a by DFT	E_a by BV	Comments
1	$LiMnPO_4$	0.31[1]	1.03	Olivine[2]
2	$LiFePO_4$	0.32[1]	0.93	Olivine[3]
3	$LiCoPO_4$	0.28[1]	0.90	Olivine[4]
4	$LiNiPO_4$	0.22[1]	0.91	Olivine[2]
5	$LiMgPO_4$	0.30[5]	0.88	Olivine[6]
6	$LiAlSiO_4$	0.20[5]	0.34	Olivine[7]
7	$LiScSiO_4$	0.33[5]	0.95	Olivine[9]
8	$LiInSiO_4$	0.40[5]	0.97	Olivine[10]
9	$LiTmSiO_4$	0.43[5]	0.98	Olivine[11]
10	$LiAlGeO_4$	0.11[5]	0.56	Olivine[12]
11	$LiInGeO_4$	0.28[5]	0.86	Olivine[13]
12	$LiScGeO_4$	0.22[5]	0.84	Olivine[14]
13	$LiMn_2O_4$	0.39[15]	0.61	Spinel[16]
14	$LiNi_{1/2}Ge_{3/2}O_4$	0.47[17]	0.67	Spinel[18]
15	$LiNi_{1/2}Mn_{3/2}O_4$	0.32[17]	0.86	Spinel[19]
16	$LiTi_2O_4$	0.28[20]	0.64	Spinel[21]
17	$Li_4Ti_5O_{12}$	0.30[22]	0.59	Spinel[23]
18	$LiCoO_2$	0.84[24]	2.15	Layer[25]
19	$LiCrO_2$	0.80[26]	1.96	Layer[27]
20	Li_2MnO_3	0.54[28]	1.08	Layer[29]
21	Li_2IrO_3	0.52[30]	1.12	Layer[31]
22	$LiTiS_2$	0.70[32]	1.93	Layer[33]
23	$LiFeSO_4OH$	0.20[34]	0.82	Layer[35]
24	$LiMnBO_3$	0.36[36]	0.57	Borate/Carbonate[37]
25	$LiFeBO_3$	0.22[36]	0.58	Borate/Carbonate[38]
26	$LiCoBO_3$	0.37[36]	0.63	Borate/Carbonate[39]
27	$LiBO_2$	0.50[40]	0.83	Borate/Carbonate[41]
28	$Li_{2.6}C_{0.33}B_{0.67}O_3$	0.21[42]	0.47	Borate/Carbonate[42]
29	Li_2CO_3	0.30[43]	0.54	Borate/Carbonate[44]
30	Li_3OCl	0.37[45]	0.98	Antiperovskite[46]
31	Li_3OBr	0.41[45]	1.29	Antiperovskite[46]
32	β-Li_3PO_4	0.39[47]	0.90	Phosphate[48]
33	γ-Li_3PO_4	0.29[47]	0.82	Phosphate[49]
34	β-Li_3PS_4	0.20[50]	0.78	Thiophosphate[51]
35	$Li_7P_3S_{11}$	0.24[52]	0.82	Thiophosphate[53]
36	$Li_2Fe(SO_4)_2$	0.47[54]	0.88	Sulphate[55]
37	$Li_2Mn(SO_4)_2$	0.54[54]	0.92	Sulphate[56]
38	$Li_2Co(SO_4)_2$	0.42[54]	0.84	Sulphate[55]
39	$LiAlPO_4F$	0.55[57]	0.88	Tavorite[58]

40	$LiMgSO_4F$	0.20[57]	0.89	Tavorite[59]
41	$LiFeSO_4F$	0.44[60]	1.02	Tavorite[61]
42	$FeSO_4F$	0.21[62]	0.60	Tavorite[62]
43	$LiTi_2(PO_4)_3$	0.25[63]	0.68	NASICON[64]
44	Li_2NiO_2	0.45[65]	0.60	Orthorhombic[66]
45	Li_2O	0.30[67]	0.63	Cubic[68]
46	LiF	0.73[69]	1.07	Cubic[70]

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