Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Rationalize the interphase stability of Li|doped-$Li_7La_3Zr_2O_{12}$ via automated reaction screening and machine learning

Bo Liu[a,b], Jiong Yang[a,*], Hongliang Yang[b,c], Caichao Ye[b], Yuanqing Mao[b], Jiping Wang[b], Siqi Shi[a], Jihui Yang[d,*], and Wenqing Zhang[b,*]

[a]Materials Genome Institute, Shanghai University, Shanghai 200444, China

[b]Department of Physics and Shenzhen Institute for Quantum Science & Technology, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China

[c]State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China

[d]Department of Materials Science and Engineering, University of Washington, Seattle, WA 98195, USA

Table S1. The complete computational results of lithiation reactions for LLZOM (M = dopants). The reaction energy ΔG is normalized to per formula-unit for the lithiation of LLZOM to form the phase equilibria with Li metal. The LLZOM compounds were thermodynamically stable against Li metal, which has a positive reaction energy value in complete lithiated process. The left side of the reaction energy column is our calculation result, and the right side is the result of MP[1] database.

System	Doped Site	Dopant	Oxidation state	Formation energy (eV/atom)	Li number	Reaction energy $\Delta G/\Delta G_{MP}$ (eV/atom)	Reaction products			
Li56La24Zr16O96				-3.128	6.667	-0.0224/-0.016	La2O3	Li2O	Zr3O	
					7.000	-0.0226/-0.016	La2O3	Li2O	Zr4O	
					8.000	-0.0216	La2O3	Li2O	Zr	
Li53La24Zr16AlO96	Li	Al	3	-3.195	0.542	0.0153	La2O3	Li2O	Li6Zr2O7	ZrAl3
					0.625	0.0143/-0.003	La2O3	Li2O	Li6Zr2O7	ZrAl2
					0.708	0.0138/-0.004	La2O3	Li2O	Li6Zr2O7	Zr2Al3
					1.042	0.0119/-0.005	La2O3	Li2O	Li6Zr2O7	Zr4Al3
					1.875	0.0096/-0.007	La2O3	Li2O	Li6Zr2O7	Zr3Al
					7.292	-0.0009/-0.014	La2O3	Li2O	Zr3O	Zr3Al
					7.563	-0.0012/-0.015	La2O3	Li2O	Zr4O	Zr3Al
					8.375	-0.0010	La2O3	Li2O	Zr	Zr3Al
					8.656	0.0016	La2O3	Li2O	Zr	Li9Al4
Li50La24Zr16Al2O96	Li	Al	3	-3.184	0.419	-0.0292	La2O3	Li5AlO4	Li6Zr2O7	ZrAl3
					1.083	-0.0315	La2O3	Li2O	Li6Zr2O7	ZrAl3
					1.250	-0.0332/-0.009	La2O3	Li2O	Li6Zr2O7	ZrAl2
					1.417	-0.0339/-0.010	La2O3	Li2O	Li6Zr2O7	Zr2Al3
					2.083	-0.0362/-0.013	La2O3	Li2O	Li6Zr2O7	Zr4Al3
					3.750	-0.0377/-0.016	La2O3	Li2O	Li6Zr2O7	Zr3Al
					7.917	-0.0394/-0.020	La2O3	Li2O	Zr3O	Zr3Al
					8.125	-0.0393/-0.020	La2O3	Li2O	Zr4O	Zr3Al
					8.750	-0.0384	La2O3	Li2O	Zr	Zr3Al
Li53La24Zr16GaO96	Li	Ga	3	-3.180	0.375	0.0042/-0.013	La2O3	Li2O	Li6Zr2O7	Ga
					0.411	0.0030/-0.015	La2O3	Li2O	Li6Zr2O7	Li2Ga7
					0.437	0.0023/-0.015	La2O3	Li2O	Li6Zr2O7	LaGa6
					0.500	0.0009/-0.017	La2O3	Li2O	Li6Zr2O7	LiGa
					0.542	0.0006	La2O3	Li2O	Li6Zr2O7	ZrGa3
					0.562	-0.0001/-0.018	La2O3	Li2O	Li6Zr2O7	LaGa2
					0.625	-0.0005	La2O3	Li2O	Li6Zr2O7	ZrGa2
					0.708	-0.0016/-0.019	La2O3	Li2O	Li6Zr2O7	Zr2Ga3
					0.875	-0.0031/-0.020	La2O3	Li2O	Li6Zr2O7	ZrGa
					1.125	-0.0040/-0.021	La2O3	Li2O	Li6Zr2O7	Zr3Ga2
					1.375	-0.0046/-0.021	La2O3	Li2O	Li6Zr2O7	Zr2Ga

					7.208	-0.0132/-0.027	La2O3	Li2O	Zr3O	Zr2Ga
					7.500	-0.0134/-0.027	La2O3	Li2O	Zr4O	Zr2Ga
					8.375	-0.0129	La2O3	Li2O	Zr	Zr2Ga
Li53La24Zr16BrO96	Li	Br	3	-3.144	0.500	-0.047/-0.060	La2O3	Li2O	Li6Zr2O7	LiBr
					7.167	-0.048/-0.058	La2O3	Li2O	Zr3O	LiBr
					7.500	-0.048/-0.057	La2O3	Li2O	Zr4O	LiBr
					8.500	-0.0461	La2O3	Li2O	Zr	LiBr
Li53La24Zr16BO96	Li	B	3	-3.190	0.625	0.0058/-0.012	La2O3	Li2O	Li6Zr2O7	ZrB2
					7.083	-0.0059/-0.019	La2O3	Li2O	Zr3O	ZrB2
					7.406	-0.0063/-0.020	La2O3	Li2O	Zr4O	ZrB2
					8.375	-0.0059	La2O3	Li2O	Zr	ZrB2
Li54La24Zr16ZnO96	Li	Zn	2	-3.165	0.250	0.0058/-0.012	La2O3	Li2O	Li6Zr2O7	Zn
					0.279	0.0049/-0.013	La2O3	Li2O	Li6Zr2O7	LaZn13
					0.284	0.0048/-0.013	La2O3	Li2O	Li6Zr2O7	LaZn11
					0.294	0.0046/-0.013	La2O3	Li2O	Li6Zr2O7	La2Zn17
					0.375	0.0036/-0.014	La2O3	Li2O	Li6Zr2O7	LiZn
					0.417	0.0036	La2O3	Li2O	Li6Zr2O7	ZrZn3
					0.500	0.0031	La2O3	Li2O	Li6Zr2O7	ZrZn2
					0.750	0.0020/-0.016	La2O3	Li2O	Li6Zr2O7	ZrZn
					7.000	-0.0086/-0.022	La2O3	Li2O	Zr3O	ZrZn
					7.312	-0.0089/-0.023	La2O3	Li2O	Zr4O	ZrZn
					8.250	-0.0084	La2O3	Li2O	Zr	ZrZn
Li54La24Zr16CdO96	Li	Cd	2	-3.158	0.250	-0.0010/-0.018	La2O3	Li2O	Li6Zr2O7	Cd
					0.292	-0.0023/-0.019	La2O3	Li2O	Li6Zr2O7	LiCd3
					0.375	-0.0037/-0.020	La2O3	Li2O	Li6Zr2O7	LiCd
					0.625	-0.0047/-0.021	La2O3	Li2O	Li6Zr2O7	Li3Cd
					7.292	-0.0145/-0.027	La2O3	Li2O	Zr3O	Li3Cd
					7.625	-0.0147/-0.027	La2O3	Li2O	Zr4O	Li3Cd
					8.625	-0.0141	La2O3	Li2O	Zr	Li3Cd
Li53La24Zr16FeO96	Li	Fe	3	-3.164	0.375	-0.0115/-0.020	La2O3	Li2O	Li6Zr2O7	Fe
					0.625	-0.0140/-0.022	La2O3	Li2O	Li6Zr2O7	ZrFe2
					1.875	-0.0158/-0.024	La2O3	Li2O	Li6Zr2O7	Zr3Fe
					7.292	-0.0219/-0.028	La2O3	Li2O	Zr3O	Zr3Fe
					7.562	-0.0220/-0.028	La2O3	Li2O	Zr4O	Zr3Fe
					8.375	-0.0213	La2O3	Li2O	Zr	Zr3Fe
Li58La23Zr16KO96	La	K	1	-3.114	0.125	0.0057/-0.003	La2O3	Li2O	Li6Zr2O7	K
					6.792	-0.0063/-0.013	La2O3	Li2O	Zr3O	K
					7.125	-0.0066/-0.013	La2O3	Li2O	Zr4O	K
					8.125	-0.0062	La2O3	Li2O	Zr	K
Li58La23Zr16NaO96	La	Na	1	-3.115	0.125	0.0067/-0.003	La2O3	Li2O	Li6Zr2O7	Na
					6.792	-0.0055/-0.013	La2O3	Li2O	Zr3O	Na

					7.125	-0.0059/-0.013	La2O3	Li2O	Zr4O	Na
					8.125	-0.0055	La2O3	Li2O	Zr	Na
Li58La23Zr16RbO96	La	Rb	1	-3.114	0.125	0.0057/-0.005	La2O3	Li2O	Li6Zr2O7	Rb
					6.792	-0.0063/-0.014	La2O3	Li2O	Zr3O	Rb
					7.125	-0.0066/-0.015	La2O3	Li2O	Zr4O	Rb
					8.125	-0.0062	La2O3	Li2O	Zr	Rb
Li58La23Zr16CsO96	La	Cs	1	-3.110	0.125	0.0018/-0.005	La2O3	Li2O	Li6Zr2O7	Cs
					6.792	-0.0094/-0.015	La2O3	Li2O	Zr3O	Cs
					7.125	-0.0097/-0.015	La2O3	Li2O	Zr4O	Cs
					8.125	-0.0092	La2O3	Li2O	Zr	Cs
Li58La23Zr16AgO96	La	Ag	1	-3.100	0.125	-0.0082/-0.012	La2O3	Li2O	Li6Zr2O7	Ag
					0.167	-0.0091/-0.013	La2O3	Li2O	Li6Zr2O7	LiAg3
					0.250	-0.0104/-0.015	La2O3	Li2O	Li6Zr2O7	LiAg
					0.325	-0.0107/-0.015	La2O3	Li2O	Li6Zr2O7	Li8Ag5
					0.500	-0.0113/-0.015	La2O3	Li2O	Li6Zr2O7	Li3Ag
					1.125	-0.0111	La2O3	Li2O	Li6Zr2O7	Zr2Ag
					6.958	-0.0185	La2O3	Li2O	Zr3O	Zr2Ag
					7.167	-0.0196/-0.023	La2O3	Li2O	Zr3O	Li3Ag
					7.500	-0.0198/-0.023	La2O3	Li2O	Zr4O	Li3Ag
					8.500	-0.0190	La2O3	Li2O	Zr	Li3Ag
Li57La23Zr16BaO96	La	Ba	2	-3.133	0.250	0.0086/-0.001	La2O3	Li2O	Li6Zr2O7	Ba
					6.917	-0.0041/-0.011	La2O3	Li2O	Zr3O	Ba
					7.250	-0.0044/-0.012	La2O3	Li2O	Zr4O	Ba
					8.250	-0.0041	La2O3	Li2O	Zr	Ba
Li57La23Zr16CaO96	La	Ca	2	-3.136	0.250	0.0116	La2O3	Li2O	Li6Zr2O7	Ca
					6.667	-0.0034/-0.011	La2O3	Li2O	Zr3O	CaO
					7.000	-0.0038/-0.011	La2O3	Li2O	Zr4O	CaO
					8.000	-0.0034	La2O3	Li2O	Zr	CaO
Li57La23Zr16SrO96	La	Sr	2	-3.136	0.250	0.0116	La2O3	Li2O	Li6Zr2O7	Sr
					6.667	-0.0016/-0.011	La2O3	Li2O	Zr3O	SrO
					7.000	-0.0020/-0.011	La2O3	Li2O	Zr4O	SrO
					7.250	-0.0021/-0.011	La2O3	Li2O	Zr4O	Sr
					7.333	-0.0021/-0.011	La2O3	Li2O	Zr4O	Sr3Li2
					8.333	-0.0018	La2O3	Li2O	Zr	Sr3Li2
Li57La23Zr16PbO96	La	Pb	2	-3.115	0.250	-0.0092/-0.017	La2O3	Li2O	Li6Zr2O7	Pb
					0.375	-0.0120/-0.019	La2O3	Li2O	Li6Zr2O7	LiPb
					0.583	-0.0151/-0.022	La2O3	Li2O	Li6Zr2O7	Li8Pb3
					0.625	-0.0156/-0.023	La2O3	Li2O	Li6Zr2O7	Li3Pb
					0.687	-0.0162/-0.024	La2O3	Li2O	Li6Zr2O7	Li7Pb2
					0.781	-0.0166/-0.024	La2O3	Li2O	Li6Zr2O7	Li17Pb4
					7.448	-0.0238/-0.029	La2O3	Li2O	Zr3O	Li17Pb4

					7.781	-0.0239/-0.029	La2O3	Li2O	Zr4O	Li17Pb4
					8.781	-0.0230	La2O3	Li2O	Zr	Li17Pb4
Li57La23Zr16CdO96	La	Cd	2	-3.112	0.250	-0.0122/-0.018	La2O3	Li2O	Li6Zr2O7	Cd
					0.292	-0.0134/-0.019	La2O3	Li2O	Li6Zr2O7	LiCd3
					0.375	-0.0147/-0.020	La2O3	Li2O	Li6Zr2O7	LiCd
					0.625	-0.0156/-0.021	La2O3	Li2O	Li6Zr2O7	Li3Cd
					7.292	-0.0230/-0.027	La2O3	Li2O	Zr3O	Li3Cd
					7.625	-0.0232/-0.027	La2O3	Li2O	Zr4O	Li3Cd
					8.625	-0.0222	La2O3	Li2O	Zr	Li3Cd
Li56La23Zr16TlO96	La	Tl	3	-3.124	0.250	-0.0068/-0.022	La2O3	Li2O	Li6Zr2O7	Tl2O
					0.375	-0.0163/-0.031	La2O3	Li2O	Li6Zr2O7	Tl
					0.500	-0.0186/-0.033	La2O3	Li2O	Li6Zr2O7	LiTl
					0.625	-0.0198/-0.035	La2O3	Li2O	Li6Zr2O7	Li2Tl
					0.687	-0.0203/-0.035	La2O3	Li2O	Li6Zr2O7	Li5Tl2
					0.750	-0.0207/-0.035	La2O3	Li2O	Li6Zr2O7	Li3Tl
					7.417	-0.0270/-0.038	La2O3	Li2O	Zr3O	Li3Tl
					7.750	-0.0271/-0.038	La2O3	Li2O	Zr4O	Li3Tl
					8.750	-0.0261	La2O3	Li2O	Zr	Li3Tl
Li56La23Zr16InO96	La	In	3	-3.134	0.375	-0.0065/-0.021	La2O3	Li2O	Li6Zr2O7	In
					0.417	-0.0073/-0.022	La2O3	Li2O	Li6Zr2O7	LiIn3
					0.500	-0.0091/-0.024	La2O3	Li2O	Li6Zr2O7	LiIn
					0.562	-0.0101/-0.025	La2O3	Li2O	Li6Zr2O7	Li3In2
					0.625	-0.0108/-0.025	La2O3	Li2O	Li6Zr2O7	Li2In
					0.917	-0.0118/-0.026	La2O3	Li2O	Li6Zr2O7	Li13In3
					1.875	-0.0134/-0.027	La2O3	Li2O	Li6Zr2O7	Zr3In
					7.292	-0.0198/-0.031	La2O3	Li2O	Zr3O	Zr3In
					7.583	-0.0200/-0.031	La2O3	Li2O	Zr3O	Li13In3
					7.917	-0.0202/-0.031	La2O3	Li2O	Zr4O	Li13In3
					8.917	-0.0194	La2O3	Li2O	Zr	Li13In3
Li56La23Zr16SbO96	La	Sb	3	-3.136	0.375	-0.0045/-0.021	La2O3	Li2O	Li6Zr2O7	Sb
					0.625	-0.0135/-0.030	La2O3	Li2O	Li6Zr2O7	La2SbO2
					0.750	-0.0172/-0.033	La2O3	Li2O	Li6Zr2O7	Li3Sb
					7.417	-0.0243/-0.037	La2O3	Li2O	Zr3O	Li3Sb
					7.750	-0.0244/-0.037	La2O3	Li2O	Zr4O	Li3Sb
					8.750	-0.0235	La2O3	Li2O	Zr	Li3Sb
Li56La23Zr16BiO96	La	Bi	3	-3.135	0.375	-0.0055/-0.025	La2O3	Li2O	Li6Zr2O7	Bi
					0.625	-0.0140/-0.033	La2O3	Li2O	Li6Zr2O7	La2BiO2
					0.750	-0.0161/-0.035	La2O3	Li2O	Li6Zr2O7	Li3Bi
					7.417	-0.0234/-0.038	La2O3	Li2O	Zr3O	Li3Bi
					7.750	-0.0235/-0.038	La2O3	Li2O	Zr4O	Li3Bi
					8.750	-0.0226	La2O3	Li2O	Zr	Li3Bi

Li56La23Zr16AcO96	La	Ac	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Ac
					6.667	0.0079/-0.011	La2O3	Li2O	Zr3O	Ac2O3
					7.000	0.0074/-0.011	La2O3	Li2O	Zr4O	Ac2O3
					8.000	0.0074	La2O3	Li2O	Zr	Ac2O3
Li56La23Zr16DyO96	La	Dy	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Dy
					6.667	0.0049/-0.011	La2O3	Li2O	Zr3O	LiDyO2
					7.000	0.0044/-0.011	La2O3	Li2O	Zr4O	LiDyO2
					8.000	0.0045	La2O3	Li2O	Zr	LiDyO2
Li56La23Zr16ErO96	La	Er	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Er
					6.667	0.0044/-0.011	La2O3	Li2O	Zr3O	LiErO2
					7.000	0.0040/-0.011	La2O3	Li2O	Zr4O	LiErO2
					8.000	0.0041	La2O3	Li2O	Zr	LiErO2
Li56La23Zr16GdO96	La	Gd	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Gd
					6.667	0.0063/-0.011	La2O3	Li2O	Zr3O	LiGdO2
					7.000	0.0058/-0.011	La2O3	Li2O	Zr4O	LiGdO2
					8.000	0.0058	La2O3	Li2O	Zr	LiGdO2
Li56La23Zr16HoO96	La	Ho	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Ho
					6.667	0.0047/-0.011	La2O3	Li2O	Zr3O	LiHoO2
					7.000	0.0043/-0.011	La2O3	Li2O	Zr4O	LiHoO2
					8.000	0.0044	La2O3	Li2O	Zr	LiHoO2
Li56La23Zr16LuO96	La	Lu	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Lu
					6.667	0.0033/-0.011	La2O3	Li2O	Zr3O	LiLuO2
					7.000	0.0029/-0.011	La2O3	Li2O	Zr4O	LiLuO2
					8.000	0.0031	La2O3	Li2O	Zr	LiLuO2
Li56La23Zr16NdO96	La	Nd	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Nd
					6.667	0.0074/-0.011	La2O3	Li2O	Zr3O	Nd2O3
					7.000	0.0069/-0.011	La2O3	Li2O	Zr4O	Nd2O3
					8.000	0.0069	La2O3	Li2O	Zr	Nd2O3
Li56La23Zr16PmO96	La	Pm	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Pm
					6.667	0.0068/-0.011	La2O3	Li2O	Zr3O	Pm2O3
					7.000	0.0064/-0.011	La2O3	Li2O	Zr4O	Pm2O3
					8.000	0.0064	La2O3	Li2O	Zr	Pm2O3
Li56La23Zr16PrO96	La	Pr	3	-3.164	0.375	0.0230	La2O3	Li2O	Li6Zr2O7	Pr
					6.667	0.0071/-0.011	La2O3	Li2O	Zr3O	Pr2O3
					7.000	0.0067/-0.011	La2O3	Li2O	Zr4O	Pr2O3
					8.000	0.0067	La2O3	Li2O	Zr	Pr2O3
Li56La23Zr16SmO96	La	Sm	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Sm
					6.667	0.0066/-0.011	La2O3	Li2O	Zr3O	Sm2O3
					7.000	0.0061/-0.011	La2O3	Li2O	Zr4O	Sm2O3
					8.000	0.0062	La2O3	Li2O	Zr	Sm2O3
Li56La23Zr16TbO96	La	Tb	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Tb

					6.667	0.0052/-0.011	La2O3	Li2O	Zr3O	LiTbO2
					7.000	0.0048/-0.011	La2O3	Li2O	Zr4O	LiTbO2
					8.000	0.0048	La2O3	Li2O	Zr	LiTbO2
Li56La23Zr16TmO96	La	Tm	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Tm
					6.667	0.0039/-0.011	La2O3	Li2O	Zr3O	LiTmO2
					7.000	0.0035/-0.011	La2O3	Li2O	Zr4O	LiTmO2
					8.000	0.0036	La2O3	Li2O	Zr	LiTmO2
Li56La23Zr16CeO96	La	Ce	3	-3.163	0.125	0.0209/-0.001	La2O3	Li2O	Li6Zr2O7	CeO
					6.792	0.0054/-0.011	La2O3	Li2O	Zr3O	CeO
					7.125	0.0050/-0.011	La2O3	Li2O	Zr4O	CeO
					8.125	0.0050	La2O3	Li2O	Zr	CeO
Li56La23Zr16YbO96	La	Yb	3	-3.150	0.125	0.0037/-0.015	La2O3	Li2O	Li6Zr2O7	YbO
					6.792	-0.0080/-0.022	La2O3	Li2O	Zr3O	YbO
					7.125	-0.0083/-0.023	La2O3	Li2O	Zr4O	YbO
					8.125	-0.0078	La2O3	Li2O	Zr	YbO
Li56La23Zr16YO96	La	Y	3	-3.165	0.375	0.0240	La2O3	Li2O	Li6Zr2O7	Y
					6.667	0.0055/-0.011	La2O3	Li2O	Zr3O	LiYO2
					7.000	0.0050/-0.011	La2O3	Li2O	Zr4O	LiYO2
					8.000	0.0051	La2O3	Li2O	Zr	LiYO2
Li56La23Zr16NO96	La	N	3	-3.109	0.375	-0.0311/-0.035	La2O3	Li2O	Li6Zr2O7	N2
					0.417	-0.0339/-0.037	La2O3	Li2O	Li6Zr2O7	LiN3
					0.750	-0.0471/-0.051	La2O3	Li2O	Li6Zr2O7	Li2ZrN2
					0.875	-0.0501/-0.054	La2O3	Li2O	Li6Zr2O7	ZrN
					1.375	-0.0514/-0.055	La2O3	Li2O	Li6Zr2O7	Zr2N
					7.208	-0.0513/-0.054	La2O3	Li2O	Zr3O	Zr2N
					7.500	-0.0511/-0.054	La2O3	Li2O	Zr4O	Zr2N
					8.375	-0.0495	La2O3	Li2O	Zr	Zr2N
Li56La23Zr16ScO96	La	Sc	3	-3.160	0.375	0.0191	La2O3	Li2O	Li6Zr2O7	Sc
					6.667	0.0001/-0.011	La2O3	Li2O	Zr3O	LiScO2
					7.000	-0.0003/-0.011	La2O3	Li2O	Zr4O	LiScO2
					8.000	0.0	La2O3	Li2O	Zr	LiScO2
Li58La24Zr15CdO96	Zr	Cd	2	-3.101	0.250	-0.0100/-0.018	La2O3	Li2O	Li6Zr2O7	Cd
					0.292	-0.0112/-0.019	La2O3	Li2O	Li6Zr2O7	LiCd3
					0.375	-0.0125/-0.020	La2O3	Li2O	Li6Zr2O7	LiCd
					0.625	-0.0134/-0.021	La2O3	Li2O	Li6Zr2O7	Li3Cd
					6.875	-0.0209/-0.027	La2O3	Li2O	Zr3O	Li3Cd
					7.187	-0.0210/-0.027	La2O3	Li2O	Zr4O	Li3Cd
					8.125	-0.0202	La2O3	Li2O	Zr	Li3Cd
Li58La24Zr15HgO96	Zr	Hg	2	-3.091	0.250	-0.0199/-0.023	La2O3	Li2O	Li6Zr2O7	Hg
					0.375	-0.0235/-0.027	La2O3	Li2O	Li6Zr2O7	LiHg
					0.625	-0.0252/-0.028	La2O3	Li2O	Li6Zr2O7	Li3Hg

					6.875	-0.0303/-0.032	La2O3	Li2O	Zr3O	Li3Hg
					7.187	-0.0303/-0.032	La2O3	Li2O	Zr4O	Li3Hg
					8.125	-0.0293	La2O3	Li2O	Zr	Li3Hg
Li58La24Zr15MgO96	Zr	Mg	2	-3.117	0.375	0.0052/-0.001	La2O3	Li2O	Li6Zr2O7	LiMg
					0.625	0.0051	La2O3	Li2O	Li6Zr2O7	Li3Mg
					0.875	0.0050	La2O3	Li2O	Li6Zr2O7	Li5Mg
					6.625	-0.0061/-0.011	La2O3	Li2O	Zr3O	LiMg
					6.937	-0.0064/-0.011	La2O3	Li2O	Zr4O	LiMg
					7.187	-0.0064/-0.011	La2O3	Li2O	Zr4O	Li3Mg
					7.437	-0.0063/-0.011	La2O3	Li2O	Zr4O	Li5Mg
					8.375	-0.0059	La2O3	Li2O	Zr	Li5Mg
Li58La24Zr15CuO96	Zr	Cu	2	-3.095	0.125	-0.0063/-0.011	La2O3	Li2O	Li6Zr2O7	LiCuO
					0.250	-0.0159/-0.020	La2O3	Li2O	Li6Zr2O7	Cu
					0.387	-0.0171/-0.022	La2O3	Li2O	Li6Zr2O7	Zr14Cu51
					1.250	-0.0190/-0.023	La2O3	Li2O	Li6Zr2O7	Zr2Cu
					6.667	-0.0245/-0.028	La2O3	Li2O	Zr3O	Zr2Cu
					6.937	-0.0246/-0.028	La2O3	Li2O	Zr4O	Zr2Cu
					7.750	-0.0238	La2O3	Li2O	Zr	Zr2Cu
Li58La24Zr15NiO96	Zr	Ni	2	-3.094	0.250	-0.0169/-0.022	La2O3	Li2O	Li6Zr2O7	Ni
					0.393	-0.0199/-0.025	La2O3	Li2O	Li6Zr2O7	Zr2Ni7
					0.417	-0.0201/-0.025	La2O3	Li2O	Li6Zr2O7	ZrNi3
					0.750	-0.0220/-0.027	La2O3	Li2O	Li6Zr2O7	ZrNi
					1.250	-0.0227/-0.028	La2O3	Li2O	Li6Zr2O7	Zr2Ni
					6.667	-0.0275/-0.031	La2O3	Li2O	Zr3O	Zr2Ni
					6.937	-0.0276/-0.031	La2O3	Li2O	Zr4O	Zr2Ni
					7.750	-0.0268	La2O3	Li2O	Zr	Zr2Ni
Li58La24Zr15EuO96	Zr	Eu	2	-3.094	0.250	-0.0169	La2O3	Li2O	Li6Zr2O7	Eu
					6.250	-0.0242/-0.010	La2O3	Li2O	Zr3O	EuO
					6.562	-0.0243/-0.010	La2O3	Li2O	Zr4O	EuO
					7.500	-0.0234	La2O3	Li2O	Zr	EuO
Li58La24Zr15CaO96	Zr	Ca	2	-3.122	0.250	0.0108	La2O3	Li2O	Li6Zr2O7	Ca
					6.250	-0.0034/-0.010	La2O3	Li2O	Zr3O	CaO
					6.562	-0.0037/-0.010	La2O3	Li2O	Zr4O	CaO
					7.500	-0.0034	La2O3	Li2O	Zr	CaO
Li58La24Zr15BeO96	Zr	Be	2	-3.115	0.288	0.0027	La2O3	Li2O	Li6Zr2O7	ZrBe13
					0.309	0.0024	La2O3	Li2O	Li6Zr2O7	Zr2Be17
					0.350	0.0022/-0.002	La2O3	Li2O	Li6Zr2O7	ZrBe5
					6.517	-0.0084/-0.011	La2O3	Li2O	Zr3O	ZrBe5
					6.825	-0.0087/-0.011	La2O3	Li2O	Zr4O	ZrBe5
					7.750	-0.0082	La2O3	Li2O	Zr	ZrBe5
Li58La24Zr15ZnO96	Zr	Zn	2	-3.104	0.250	-0.0070/-0.012	La2O3	Li2O	Li6Zr2O7	Zn

					0.279	-0.0079/-0.013	La2O3	Li2O	Li6Zr2O7	LaZn13
					0.284	-0.0081/-0.013	La2O3	Li2O	Li6Zr2O7	LaZn11
					0.294	-0.0082/-0.013	La2O3	Li2O	Li6Zr2O7	La2Zn17
					0.375	-0.0091/-0.014	La2O3	Li2O	Li6Zr2O7	LiZn
					0.417	-0.0092	La2O3	Li2O	Li6Zr2O7	ZrZn3
					0.500	-0.0096	La2O3	Li2O	Li6Zr2O7	ZrZn2
					0.750	-0.0105/-0.015	La2O3	Li2O	Li6Zr2O7	ZrZn
					6.583	-0.0181/-0.022	La2O3	Li2O	Zr3O	ZrZn
					6.875	-0.0183/-0.022	La2O3	Li2O	Zr4O	ZrZn
					7.750	-0.0176	La2O3	Li2O	Zr	ZrZn
Li58La24Zr15MnO96	Zr	Mn	2	-3.093	0.250	-0.0179/-0.011	La2O3	Li2O	Li6Zr2O7	Mn
					0.500	-0.0196/-0.013	La2O3	Li2O	Li6Zr2O7	ZrMn2
					6.542	-0.0256/-0.020	La2O3	Li2O	Zr3O	ZrMn2
					6.844	-0.0258/-0.020	La2O3	Li2O	Zr4O	ZrMn2
					7.750	-0.0248	La2O3	Li2O	Zr	ZrMn2
Li58La24Zr15SrO96	Zr	Sr	2	-3.118	0.250	0.0068	La2O3	Li2O	Li6Zr2O7	Sr
					6.250	-0.0047/-0.010	La2O3	Li2O	Zr3O	SrO
					6.562	-0.0051/-0.010	La2O3	Li2O	Zr4O	SrO
					6.812	-0.0052/-0.010	La2O3	Li2O	Zr4O	Sr
					6.896	-0.0051/-0.010	La2O3	Li2O	Zr4O	Sr3Li2
					7.833	-0.0048	La2O3	Li2O	Zr	Sr3Li2
Li58La24Zr15FeO96	Zr	Fe	2	-3.093	0.250	-0.0179/-0.013	La2O3	Li2O	Li6Zr2O7	Fe
					0.500	-0.0203/-0.016	La2O3	Li2O	Li6Zr2O7	ZrFe2
					1.750	-0.0218/-0.017	La2O3	Li2O	Li6Zr2O7	Zr3Fe
					6.750	-0.0264/-0.022	La2O3	Li2O	Zr3O	Zr3Fe
					7.000	-0.0265/-0.022	La2O3	Li2O	Zr4O	Zr3Fe
					7.750	-0.0257	La2O3	Li2O	Zr	Zr3Fe
Li58La24Zr15CoO96	Zr	Co	2	-3.095	0.250	-0.0159/-0.017	La2O3	Li2O	Li6Zr2O7	Co
					0.380	-0.0175/-0.018	La2O3	Li2O	Li6Zr2O7	Zr6Co23
					0.500	-0.0185/-0.019	La2O3	Li2O	Li6Zr2O7	ZrCo2
					0.750	-0.0193/-0.020	La2O3	Li2O	Li6Zr2O7	ZrCo
					1.250	-0.0208/-0.022	La2O3	Li2O	Li6Zr2O7	Zr2Co
					1.750	-0.0215/-0.022	La2O3	Li2O	Li6Zr2O7	Zr3Co
					6.750	-0.0262/-0.027	La2O3	Li2O	Zr3O	Zr3Co
					7.000	-0.0263/-0.027	La2O3	Li2O	Zr4O	Zr3Co
					7.750	-0.0255	La2O3	Li2O	Zr	Zr3Co
Li57La24Zr15FeO96	Zr	Fe	3	-3.125	0.375	-0.0022/-0.020	La2O3	Li2O	Li6Zr2O7	Fe
					0.625	-0.0047/-0.022	La2O3	Li2O	Li6Zr2O7	ZrFe2
					1.875	-0.0070/-0.023	La2O3	Li2O	Li6Zr2O7	Zr3Fe
					6.875	-0.0140/-0.027	La2O3	Li2O	Zr3O	Zr3Fe
					7.125	-0.0142/-0.028	La2O3	Li2O	Zr4O	Zr3Fe

					7.875	-0.0137	La2O3	Li2O	Zr	Zr3Fe
Li57La24Zr15InO96	Zr	In	3	-3.127	0.417	-0.0011/-0.022	La2O3	Li2O	Li6Zr2O7	LiIn3
					0.500	-0.0028/-0.024	La2O3	Li2O	Li6Zr2O7	LiIn
					0.562	-0.0039/-0.025	La2O3	Li2O	Li6Zr2O7	Li3In2
					0.625	-0.0046/-0.025	La2O3	Li2O	Li6Zr2O7	Li2In
					0.917	-0.0057/-0.026	La2O3	Li2O	Li6Zr2O7	Li13In3
					1.875	-0.0074/-0.027	La2O3	Li2O	Li6Zr2O7	Zr3In
					6.875	-0.0144/-0.030	La2O3	Li2O	Zr3O	Zr3In
					7.167	-0.0146/-0.031	La2O3	Li2O	Zr3O	Li13In3
					7.479	-0.0149/-0.031	La2O3	Li2O	Zr4O	Li13In3
					8.417	-0.0142	La2O3	Li2O	Zr	Li13In3
Li57La24Zr15RhO96	Zr	Rh	3	-3.115	0.375	-0.0120/-0.031	La2O3	Li2O	Li6Zr2O7	Rh
					0.542	-0.0168/-0.035	La2O3	Li2O	Li6Zr2O7	ZrRh3
					0.675	-0.0189/-0.037	La2O3	Li2O	Li6Zr2O7	Zr3Rh5
					0.875	-0.0207/-0.039	La2O3	Li2O	Li6Zr2O7	ZrRh
					1.375	-0.0214/-0.039	La2O3	Li2O	Li6Zr2O7	Zr2Rh
					6.792	-0.0265/-0.041	La2O3	Li2O	Zr3O	Zr2Rh
					7.062	-0.0266/-0.041	La2O3	Li2O	Zr4O	Zr2Rh
					7.875	-0.0257	La2O3	Li2O	Zr	Zr2Rh
Li57La24Zr15ScO96	Zr	Sc	3	-3.154	0.375	0.0264	La2O3	Li2O	Li6Zr2O7	Sc
					6.250	0.0067/-0.010	La2O3	Li2O	Zr3O	LiScO2
					6.562	0.0063/-0.010	La2O3	Li2O	Zr4O	LiScO2
					7.500	0.0063	La2O3	Li2O	Zr	LiScO2
Li57La24Zr15TlO96	Zr	Tl	3	-3.115	0.250	-0.0025/-0.022	La2O3	Li2O	Li6Zr2O7	Tl2O
					0.375	-0.0120/-0.031	La2O3	Li2O	Li6Zr2O7	Tl
					0.500	-0.0143/-0.033	La2O3	Li2O	Li6Zr2O7	LiTl
					0.625	-0.0155/-0.034	La2O3	Li2O	Li6Zr2O7	Li2Tl
					0.687	-0.0160/-0.035	La2O3	Li2O	Li6Zr2O7	Li5Tl2
					0.750	-0.0164/-0.035	La2O3	Li2O	Li6Zr2O7	Li3Tl
					7.000	-0.0233/-0.038	La2O3	Li2O	Zr3O	Li3Tl
					7.312	-0.0234/-0.038	La2O3	Li2O	Zr4O	Li3Tl
					8.250	-0.0225	La2O3	Li2O	Zr	Li3Tl
Li57La24Zr15AuO96	Zr	Au	3	-3.106	0.375	-0.0209/-0.034	La2O3	Li2O	Li6Zr2O7	Au
					0.417	-0.0233/-0.037	La2O3	Li2O	Li6Zr2O7	LiAu3
					0.500	-0.0264/-0.040	La2O3	Li2O	Li6Zr2O7	LiAu
					0.750	-0.0287/-0.042	La2O3	Li2O	Li6Zr2O7	Li3Au
					0.844	-0.0288/-0.042	La2O3	Li2O	Li6Zr2O7	Li15Au4
					7.094	-0.0332/-0.043	La2O3	Li2O	Zr3O	Li15Au4
					7.406	-0.0332/-0.043	La2O3	Li2O	Zr4O	Li15Au4
					8.344	-0.0321	La2O3	Li2O	Zr	Li15Au4
Li57La24Zr15CrO96	Zr	Cr	3	-3.125	0.375	-0.0022/-0.014	La2O3	Li2O	Li6Zr2O7	Cr

					0.625	-0.0029/-0.015	La2O3	Li2O	Li6Zr2O7	ZrCr2
					6.667	-0.0123/-0.022	La2O3	Li2O	Zr3O	ZrCr2
					6.969	-0.0125/-0.022	La2O3	Li2O	Zr4O	ZrCr2
					7.875	-0.0120	La2O3	Li2O	Zr	ZrCr2
Li57La24Zr15PO96	Zr	P	3	-3.127	0.750	-0.0145/-0.021	La2O3	Li2O	Li6Zr2O7	Li3LaP2
					1.153	-0.0171/-0.023	La2O3	Li2O	Li6Zr2O7	Zr14P9
					1.250	-0.0175/-0.024	La2O3	Li2O	Li6Zr2O7	Zr7P4
					1.875	-0.0196/-0.026	La2O3	Li2O	Li6Zr2O7	Zr3P
					6.875	-0.0246/-0.029	La2O3	Li2O	Zr3O	Zr3P
					7.125	-0.0247/-0.030	La2O3	Li2O	Zr4O	Zr3P
					7.875	-0.0240	La2O3	Li2O	Zr	Zr3P
Li57La24Zr15AlO96	Zr	Al	3	-3.145	0.542	0.0138	La2O3	Li2O	Li6Zr2O7	ZrAl3
					0.625	0.0128/-0.003	La2O3	Li2O	Li6Zr2O7	ZrAl2
					0.708	0.0123/-0.004	La2O3	Li2O	Li6Zr2O7	Zr2Al3
					1.042	0.0105/-0.005	La2O3	Li2O	Li6Zr2O7	Zr4Al3
					1.875	0.0083/-0.007	La2O3	Li2O	Li6Zr2O7	Zr3Al
					6.875	-0.0012/-0.014	La2O3	Li2O	Zr3O	Zr3Al
					7.125	-0.0015/-0.014	La2O3	Li2O	Zr4O	Zr3Al
					7.875	-0.0013	La2O3	Li2O	Zr	Zr3Al
Li57La24Zr15GaO96	Zr	Ga	3	-3.129	0.375	0.0017/-0.013	La2O3	Li2O	Li6Zr2O7	Ga
					0.411	0.0006/-0.014	La2O3	Li2O	Li6Zr2O7	Li2Ga7
					0.437	-0.0001/-0.015	La2O3	Li2O	Li6Zr2O7	LaGa6
					0.500	-0.0015/-0.016	La2O3	Li2O	Li6Zr2O7	LiGa
					0.562	-0.0025/-0.017	La2O3	Li2O	Li6Zr2O7	LaGa2
					0.708	-0.0040/-0.019	La2O3	Li2O	Li6Zr2O7	Zr2Ga3
					0.875	-0.0054/-0.020	La2O3	Li2O	Li6Zr2O7	ZrGa
					1.125	-0.0063/-0.021	La2O3	Li2O	Li6Zr2O7	Zr3Ga2
					1.375	-0.0068/-0.021	La2O3	Li2O	Li6Zr2O7	Zr2Ga
					6.792	-0.0145/-0.026	La2O3	Li2O	Zr3O	Zr2Ga
					7.062	-0.0147/-0.026	La2O3	Li2O	Zr4O	Zr2Ga
					7.875	-0.0141	La2O3	Li2O	Zr	Zr2Ga
Li57La24Zr15TmO96	Zr	Tm	3	-3.155	0.375	0.0273	La2O3	Li2O	Li6Zr2O7	Tm
					6.250	0.0074/-0.010	La2O3	Li2O	Zr3O	LiTmO2
					6.562	0.0070/-0.010	La2O3	Li2O	Zr4O	LiTmO2
					7.500	0.0070	La2O3	Li2O	Zr	LiTmO2
Li57La24Zr15DyO96	Zr	Dy	3	-3.153	0.375	0.0254	La2O3	Li2O	Li6Zr2O7	Dy
					6.250	0.0068/-0.010	La2O3	Li2O	Zr3O	LiDyO2
					6.562	0.0064/-0.010	La2O3	Li2O	Zr4O	LiDyO2
					7.500	0.0064	La2O3	Li2O	Zr	LiDyO2
Li57La24Zr15BiO96	Zr	Bi	3	-3.120	0.375	-0.0071/-0.025	La2O3	Li2O	Li6Zr2O7	Bi
					0.625	-0.0156/-0.033	La2O3	Li2O	Li6Zr2O7	La2BiO2

					0.750	-0.0176/-0.035	La2O3	Li2O	Li6Zr2O7	Li3Bi
					7.000	-0.0242/-0.038	La2O3	Li2O	Zr3O	Li3Bi
					7.312	-0.0243/-0.038	La2O3	Li2O	Zr4O	Li3Bi
					8.250	-0.0234	La2O3	Li2O	Zr	Li3Bi
Li57La24Zr15YO96	Zr	Y	3	-3.154	0.375	0.0264	La2O3	Li2O	Li6Zr2O7	Y
					6.250	0.0082/-0.010	La2O3	Li2O	Zr3O	LiYO2
					6.562	0.0077/-0.010	La2O3	Li2O	Zr4O	LiYO2
					7.500	0.0077	La2O3	Li2O	Zr	LiYO2
Li57La24Zr15TbO96	Zr	Tb	3	-3.153	0.375	0.0254	La2O3	Li2O	Li6Zr2O7	Tb
					6.250	0.0071/-0.010	La2O3	Li2O	Zr3O	LiTbO2
					6.562	0.0067/-0.010	La2O3	Li2O	Zr4O	LiTbO2
					7.500	0.0067	La2O3	Li2O	Zr	LiTbO2
Li57La24Zr15NdO96	Zr	Nd	3	-3.149	0.375	0.0214	La2O3	Li2O	Li6Zr2O7	Nd
					6.250	0.0062/-0.010	La2O3	Li2O	Zr3O	Nd2O3
					6.562	0.0057/-0.010	La2O3	Li2O	Zr4O	Nd2O3
					7.500	0.0058	La2O3	Li2O	Zr	Nd2O3
Li57La24Zr15SmO96	Zr	Sm	3	-3.150	0.375	0.0224	La2O3	Li2O	Li6Zr2O7	Sm
					6.250	0.0061/-0.010	La2O3	Li2O	Zr3O	Sm2O3
					6.562	0.0057/-0.010	La2O3	Li2O	Zr4O	Sm2O3
					7.500	0.0057	La2O3	Li2O	Zr	Sm2O3
Li57La24Zr15PmO96	Zr	Pm	3	-3.150	0.375	0.0224	La2O3	Li2O	Li6Zr2O7	Pm
					6.250	0.0064/-0.010	La2O3	Li2O	Zr3O	Pm2O3
					6.562	0.0060/-0.010	La2O3	Li2O	Zr4O	Pm2O3
					7.500	0.0060	La2O3	Li2O	Zr	Pm2O3
Li57La24Zr15CeO96	Zr	Ce	3	-3.147	0.125	0.0183/-0.001	La2O3	Li2O	Li6Zr2O7	CeO
					6.375	0.0042/-0.011	La2O3	Li2O	Zr3O	CeO
					6.687	0.0038/-0.011	La2O3	Li2O	Zr4O	CeO
					7.625	0.0039	La2O3	Li2O	Zr	CeO
Li57La24Zr15IrO96	Zr	Ir	3	-3.112	0.375	-0.0150/-0.031	La2O3	Li2O	Li6Zr2O7	Ir
					0.542	-0.0199/-0.036	La2O3	Li2O	Li6Zr2O7	ZrIr3
					0.875	-0.0240/-0.040	La2O3	Li2O	Li6Zr2O7	ZrIr
					1.208	-0.0255/-0.041	La2O3	Li2O	Li6Zr2O7	Zr5Ir3
					1.875	-0.0266/-0.042	La2O3	Li2O	Li6Zr2O7	Zr3Ir
					6.875	-0.0304/-0.043	La2O3	Li2O	Zr3O	Zr3Ir
					7.125	-0.0305/-0.043	La2O3	Li2O	Zr4O	Zr3Ir
					7.875	-0.0296	La2O3	Li2O	Zr	Zr3Ir
Li57La24Zr15HoO96	Zr	Ho	3	-3.154	0.375	0.0264	La2O3	Li2O	Li6Zr2O7	Ho
					6.250	0.0074/-0.010	La2O3	Li2O	Zr3O	LiHoO2
					6.562	0.0070/-0.010	La2O3	Li2O	Zr4O	LiHoO2
					7.500	0.0070	La2O3	Li2O	Zr	LiHoO2
Li57La24Zr15ErO96	Zr	Er	3	-3.154	0.375	0.0264	La2O3	Li2O	Li6Zr2O7	Er

					6.250	0.0071/-0.010	La2O3	Li2O	Zr3O	LiErO2
					6.562	0.0067/-0.010	La2O3	Li2O	Zr4O	LiErO2
					7.500	0.0067	La2O3	Li2O	Zr	LiErO2
Li57La24Zr15GdO96	Zr	Gd	3	-3.152	0.375	0.0244	La2O3	Li2O	Li6Zr2O7	Gd
					6.250	0.0074/-0.010	La2O3	Li2O	Zr3O	LiGdO2
					6.562	0.0069/-0.010	La2O3	Li2O	Zr4O	LiGdO2
					7.500	0.0069	La2O3	Li2O	Zr	LiGdO2
Li57La24Zr15RuO96	Zr	Ru	3	-3.113	0.375	-0.0140/-0.028	La2O3	Li2O	Li6Zr2O7	Ru
					0.875	-0.0211/-0.035	La2O3	Li2O	Li6Zr2O7	ZrRu
					6.708	-0.0267/-0.038	La2O3	Li2O	Zr3O	ZrRu
					7.000	-0.0268/-0.038	La2O3	Li2O	Zr4O	ZrRu
					7.875	-0.0259	La2O3	Li2O	Zr	ZrRu
Li56La24Zr15CO96	Zr	C	4	-3.089	0.500	-0.0534/-0.026	La2O3	Li2O	Li6Zr2O7	C
					1.000	-0.0613/-0.034	La2O3	Li2O	Li6Zr2O7	ZrC
					1.056	-0.0616/-0.035	La2O3	Li2O	Li6Zr2O7	Zr10C9
					6.843	-0.0595/-0.037	La2O3	Li2O	Zr3O	Zr10C9
					7.132	-0.0593/-0.037	La2O3	Li2O	Zr4O	Zr10C9
					8.000	-0.0575	La2O3	Li2O	Zr	Zr10C9
Li56La24Zr15GeO96	Zr	Ge	4	-3.099	0.500	-0.0436/-0.021	La2O3	Li2O	Li6Zr2O7	Ge
					0.625	-0.0462	La2O3	Li2O	Li6Zr2O7	LiGe
					0.705	-0.0479	La2O3	Li2O	Li6Zr2O7	La6Ge11
					0.750	-0.0492/-0.027	La2O3	Li2O	Li6Zr2O7	LiLaGe2
					1.000	-0.0516	La2O3	Li2O	Li6Zr2O7	ZrGe
					1.125	-0.0530/-0.031	La2O3	Li2O	Li6Zr2O7	Zr5Ge4
					1.333	-0.0541/-0.032	La2O3	Li2O	Li6Zr2O7	Zr5Ge3
					2.000	-0.0541/-0.032	La2O3	Li2O	Li6Zr2O7	Zr3Ge
					7.000	-0.0535/-0.035	La2O3	Li2O	Zr3O	Zr3Ge
					7.250	-0.0534/-0.035	La2O3	Li2O	Zr4O	Zr3Ge
					8.000	-0.0519	La2O3	Li2O	Zr	Zr3Ge
Li56La24Zr15HfO96	Zr	Hf	4	-3.131	0.500	-0.0123	La2O3	Li2O	Li6Zr2O7	Hf
					1.000	-0.0128	La2O3	Li2O	Li6Zr2O7	HfZr
					6.250	-0.0228/-0.010	La2O3	Li2O	Zr3O	Li6Hf2O7
					6.562	-0.0230/-0.010	La2O3	Li2O	Zr4O	Li6Hf2O7
					7.500	-0.0221	La2O3	Li2O	Zr	Li6Hf2O7
Li56La24Zr15MoO96	Zr	Mo	4	-3.097	0.500	-0.0456/-0.027	La2O3	Li2O	Li6Zr2O7	Mo
					0.750	-0.0465/-0.028	La2O3	Li2O	Li6Zr2O7	ZrMo2
					6.792	-0.0473/-0.032	La2O3	Li2O	Zr3O	ZrMo2
					7.094	-0.0472/-0.032	La2O3	Li2O	Zr4O	ZrMo2
					8.000	-0.0456	La2O3	Li2O	Zr	ZrMo2
Li56La24Zr15PbO96	Zr	Pb	4	-3.088	0.250	-0.0382/-0.022	La2O3	Li2O	Li6Zr2O7	PbO
					0.500	-0.0544/-0.038	La2O3	Li2O	Li6Zr2O7	Pb

					0.625	-0.0569/-0.041	La2O3	Li2O	Li6Zr2O7	LiPb
					0.833	-0.0596/-0.044	La2O3	Li2O	Li6Zr2O7	Li8Pb3
					0.875	-0.0600/-0.044	La2O3	Li2O	Li6Zr2O7	Li3Pb
					0.937	-0.0605/-0.045	La2O3	Li2O	Li6Zr2O7	Li7Pb2
					1.031	-0.0608/-0.045	La2O3	Li2O	Li6Zr2O7	Li17Pb4
					7.281	-0.0587/-0.046	La2O3	Li2O	Zr3O	Li17Pb4
					7.594	-0.0585/-0.046	La2O3	Li2O	Zr4O	Li17Pb4
					8.531	-0.0566	La2O3	Li2O	Zr	Li17Pb4
Li56La24Zr15PdO96	Zr	Pd	4	-3.081	0.250	-0.0400/-0.024	La2O3	Li2O	Li6Zr2O7	Li2PdO2
					0.500	-0.0612/-0.045	La2O3	Li2O	Li6Zr2O7	Pd
					0.518	-0.0622/-0.046	La2O3	Li2O	Li6Zr2O7	LiPd7
					0.575	-0.0642/-0.048	La2O3	Li2O	Li6Zr2O7	LaPd5
					0.625	-0.0658/-0.050	La2O3	Li2O	Li6Zr2O7	LaPd3
					0.667	-0.0666/-0.050	La2O3	Li2O	Li6Zr2O7	ZrPd3
					1.000	-0.0673/-0.051	La2O3	Li2O	Li6Zr2O7	ZrPd
					1.500	-0.0677/-0.052	La2O3	Li2O	Li6Zr2O7	Zr2Pd
					6.917	-0.0647/-0.051	La2O3	Li2O	Zr3O	Zr2Pd
					7.187	-0.0644/-0.051	La2O3	Li2O	Zr4O	Zr2Pd
					8.000	-0.0626	La2O3	Li2O	Zr	Zr2Pd
Li56La24Zr15PtO96	Zr	Pt	4	-3.083	0.500	-0.0593/-0.043	La2O3	Li2O	Li6Zr2O7	Pt
					0.518	-0.0607/-0.044	La2O3	Li2O	Li6Zr2O7	LiPt7
					0.542	-0.0620/-0.046	La2O3	Li2O	Li6Zr2O7	LiPt3
					0.575	-0.0634/-0.047	La2O3	Li2O	Li6Zr2O7	LaPt5
					0.625	-0.0651/-0.049	La2O3	Li2O	Li6Zr2O7	LiPt
					0.667	-0.0661/-0.050	La2O3	Li2O	Li6Zr2O7	ZrPt3
					0.812	-0.0678/-0.052	La2O3	Li2O	Li6Zr2O7	LiZrPt2
					1.000	-0.0698/-0.054	La2O3	Li2O	Li6Zr2O7	ZrPt
					6.833	-0.0661/-0.053	La2O3	Li2O	Zr3O	ZrPt
					7.125	-0.0659/-0.053	La2O3	Li2O	Zr4O	ZrPt
					8.000	-0.0639	La2O3	Li2O	Zr	ZrPt
Li56La24Zr15SO96	Zr	S	4	-3.088	0.667	-0.0658	La2O3	Li2O	Li6Zr2O7	ZrS3
					0.750	-0.0780/-0.048	La2O3	Li2O	Li6Zr2O7	La2SO2
					7.000	-0.0724/-0.048	La2O3	Li2O	Zr3O	La2SO2
					7.312	-0.0721/-0.048	La2O3	Li2O	Zr4O	La2SO2
					8.250	-0.0698	La2O3	Li2O	Zr	La2SO2
Li56La24Zr15SiO96	Zr	Si	4	-3.112	0.750	-0.0359	La2O3	Li2O	Li6Zr2O7	ZrSi2
					1.000	-0.0404/-0.013	La2O3	Li2O	Li6Zr2O7	ZrSi
					1.125	-0.0413	La2O3	Li2O	Li6Zr2O7	Zr5Si4
					1.250	-0.0422/-0.015	La2O3	Li2O	Li6Zr2O7	Zr3Si2
					1.500	-0.0428/-0.016	La2O3	Li2O	Li6Zr2O7	Zr2Si
					6.917	-0.0441/-0.022	La2O3	Li2O	Zr3O	Zr2Si

					7.187	-0.0441/-0.022	La2O3	Li2O	Zr4O	Zr2Si
					8.000	-0.0428	La2O3	Li2O	Zr	Zr2Si
Li56La24Zr15SnO96	Zr	Sn	4	-3.100	0. 500	-0.0426/-0.025	La2O3	Li2O	Li6Zr2O7	Sn
					0.625	-0.0457/-0.029	La2O3	Li2O	Li6Zr2O7	LiSn
					0.825	-0.0494/-0.032	La2O3	Li2O	Li6Zr2O7	Li13Sn5
					0.937	-0.0503/-0.033	La2O3	Li2O	Li6Zr2O7	Li7Sn2
					1.031	-0.0509/-0.034	La2O3	Li2O	Li6Zr2O7	Li17Sn4
					7.281	-0.0508/-0.037	La2O3	Li2O	Zr3O	Li17Sn4
					7.594	-0.0507/-0.037	La2O3	Li2O	Zr4O	Li17Sn4
					8.531	-0.0491	La2O3	Li2O	Zr	Li17Sn4
Li56La24Zr15TeO96	Zr	Te	4	-3.090	0.750	-0.0687/-0.048	La2O3	Li2O	Li6Zr2O7	La2TeO2
					7.000	-0.0650/-0.048	La2O3	Li2O	Zr3O	La2TeO2
					7.312	-0.0647/-0.048	La2O3	Li2O	Zr4O	La2TeO2
					8.250	-0.0627	La2O3	Li2O	Zr	La2TeO2
Li56La24Zr15TiO96	Zr	Ti	4	-3.123	0.417	-0.0203/-0.002	La2O3	Li2O	Li6Zr2O7	Ti3O
					0.625	-0.0209/-0.003	La2O3	Li2O	Li6Zr2O7	ZrTi2O
					6.667	-0.0267/-0.012	La2O3	Li2O	Zr3O	ZrTi2O
					6.969	-0.0268/-0.012	La2O3	Li2O	Zr4O	ZrTi2O
					7.875	-0.0259	La2O3	Li2O	Zr	ZrTi2O
Li56La24Zr15IrO96	Zr	Ir	4	-3.082	0.500	-0.0603/-0.042	La2O3	Li2O	Li6Zr2O7	Ir
					0.667	-0.0649/-0.047	La2O3	Li2O	Li6Zr2O7	ZrIr3
					1.000	-0.0684/-0.050	La2O3	Li2O	Li6Zr2O7	ZrIr
					1.333	-0.0693/-0.051	La2O3	Li2O	Li6Zr2O7	Zr5Ir3
					2.000	-0.0692/-0.052	La2O3	Li2O	Li6Zr2O7	Zr3Ir
					7.000	-0.0662/-0.051	La2O3	Li2O	Zr3O	Zr3Ir
					7.250	-0.0660/-0.051	La2O3	Li2O	Zr4O	Zr3Ir
					8.000	-0.0643	La2O3	Li2O	Zr	Zr3Ir
Li56La24Zr15SeO96	Zr	Se	4	-3.085	0.667	-0.0705/-0.052	La2O3	Li2O	Li6Zr2O7	La4Se3O4
					0.750	-0.0759/-0.058	La2O3	Li2O	Li6Zr2O7	La2SeO2
					7.000	-0.0708/-0.056	La2O3	Li2O	Zr3O	La2SeO2
					7.312	-0.0705/-0.056	La2O3	Li2O	Zr4O	La2SeO2
					8.250	-0.0682	La2O3	Li2O	Zr	La2SeO2
Li56La24Zr15MnO96	Zr	Mn	4	-3.086	0.125	-0.0375/-0.009	La2O3	Li2O	Li6Zr2O7	LiMnO2
					0.250	-0.0457/-0.017	La2O3	Li2O	Li6Zr2O7	Li6MnO4
					0.500	-0.0563/-0.028	La2O3	Li2O	Li6Zr2O7	Mn
					0.750	-0.0576/-0.030	La2O3	Li2O	Li6Zr2O7	ZrMn2
					6.792	-0.0562/-0.034	La2O3	Li2O	Zr3O	ZrMn2
					7.094	-0.0560/-0.034	La2O3	Li2O	Zr4O	ZrMn2
					8.000	-0.0542	La2O3	Li2O	Zr	ZrMn2
Li56La24Zr15WO96	Zr	W	4	-3.094	0.500	-0.0485/-0.025	La2O3	Li2O	Li6Zr2O7	W
					0.750	-0.0494/-0.026	La2O3	Li2O	Li6Zr2O7	ZrW2

					6.792	-0.0496/-0.031	La2O3	Li2O	Zr3O	ZrW2
					7.094	-0.0495/-0.031	La2O3	Li2O	Zr4O	ZrW2
					8.000	-0.0479	La2O3	Li2O	Zr	ZrW2
Li56La24Zr15CoO96	Zr	Co	4	-3.082	0.125	-0.0344/-0.014	La2O3	Li2O	Li6Zr2O7	Li5CoO4
					0.250	-0.0438/-0.023	La2O3	Li2O	Li6Zr2O7	Li6CoO4
					0.500	-0.0603/-0.040	La2O3	Li2O	Li6Zr2O7	Co
					0.630	-0.0616/-0.041	La2O3	Li2O	Li6Zr2O7	Zr6Co23
					0.750	-0.0624/-0.042	La2O3	Li2O	Li6Zr2O7	ZrCo2
					1.000	-0.0627/-0.043	La2O3	Li2O	Li6Zr2O7	ZrCo
					1.500	-0.0633/-0.044	La2O3	Li2O	Li6Zr2O7	Zr2Co
					2.000	-0.0633/-0.044	La2O3	Li2O	Li6Zr2O7	Zr3Co
					7.000	-0.0612/-0.045	La2O3	Li2O	Zr3O	Zr3Co
					7.250	-0.0610/-0.045	La2O3	Li2O	Zr4O	Zr3Co
					8.000	-0.0594	La2O3	Li2O	Zr	Zr3Co
Li56La24Zr15CeO96	Zr	Ce	4	-3.163	0.045	0.0202/-0.002	La2O3	Li2O	Li6Zr2O7	Ce11O20
					0.050	0.0201/-0.002	La2O3	Li2O	Li6Zr2O7	Ce5O9
					0.071	0.0194/-0.003	La2O3	Li2O	Li6Zr2O7	Ce7O12
					0.125	0.0188/-0.004	La2O3	Li2O	Li6Zr2O7	Ce2O3
					0.250	0.0179/-0.004	La2O3	Li2O	Li6Zr2O7	CeO
					6.500	0.0039/-0.013	La2O3	Li2O	Zr3O	CeO
					6.812	0.0035/-0.014	La2O3	Li2O	Zr4O	CeO
					7.750	0.0035	La2O3	Li2O	Zr	CeO
Li56La24Zr15ThO96	Zr	Th	4	-3.167	0.500	0.0230	La2O3	Li2O	Li6Zr2O7	Th
					6.250	0.0005/-0.010	La2O3	Li2O	Zr3O	La2Th8O19
					6.562	0.0001/-0.010	La2O3	Li2O	Zr4O	La2Th8O19
					7.500	0.0003	La2O3	Li2O	Zr	La2Th8O19
Li56La24Zr15UO96	Zr	U	4	-3.158	0.500	0.0142/-0.005	La2O3	Li2O	Li6Zr2O7	U
					6.750	0.0010/-0.014	La2O3	Li2O	Zr3O	U
					7.062	0.0006/-0.014	La2O3	Li2O	Zr4O	U
					8.000	0.0008	La2O3	Li2O	Zr	U
Li56La24Zr15RuO96	Zr	Ru	4	-3.122	0.500	-0.0211/-0.038	La2O3	Li2O	Li6Zr2O7	Ru
					1.000	-0.0280/-0.044	La2O3	Li2O	Li6Zr2O7	ZrRu
					6.833	-0.0323/-0.045	La2O3	Li2O	Zr3O	ZrRu
					7.125	-0.0323/-0.045	La2O3	Li2O	Zr4O	ZrRu
					8.000	-0.0313	La2O3	Li2O	Zr	ZrRu
Li56La24Zr15TcO96	Zr	Tc	4	-3.127	0.500	-0.0162/-0.031	La2O3	Li2O	Li6Zr2O7	Tc
					0.750	-0.0189/-0.034	La2O3	Li2O	Li6Zr2O7	ZrTc2
					1.625	-0.0206/-0.035	La2O3	Li2O	Li6Zr2O7	LiZr2Tc
					7.042	-0.0258/-0.037	La2O3	Li2O	Zr3O	LiZr2Tc
					7.312	-0.0259/-0.037	La2O3	Li2O	Zr4O	LiZr2Tc
					8.125	-0.0251	La2O3	Li2O	Zr	LiZr2Tc

Li56La24Zr15ReO96	Zr	Re	4	-3.124	0.500	-0.0191/-0.027	La2O3	Li2O	Li6Zr2O7	Re
					0.604	-0.0206/-0.029	La2O3	Li2O	Li6Zr2O7	Zr5Re24
					0.750	-0.0221/-0.030	La2O3	Li2O	Li6Zr2O7	ZrRe2
					0.920	-0.0227/-0.031	La2O3	Li2O	Li6Zr2O7	Zr21Re25
					6.820	-0.0280/-0.034	La2O3	Li2O	Zr3O	Zr21Re25
					7.115	-0.0281/-0.034	La2O3	Li2O	Zr4O	Zr21Re25
					8.000	-0.0272	La2O3	Li2O	Zr	Zr21Re25
Li56La24Zr15OsO96	Zr	Os	4	-3.119	0.500	-0.0240/-0.037	La2O3	Li2O	Li6Zr2O7	Os
					0.750	-0.0272/-0.040	La2O3	Li2O	Li6Zr2O7	ZrOs2
					1.000	-0.0297/-0.042	La2O3	Li2O	Li6Zr2O7	ZrOs
					1.625	-0.0309/-0.043	La2O3	Li2O	Li6Zr2O7	LiZr2Os
					7.042	-0.0343/-0.044	La2O3	Li2O	Zr3O	LiZr2Os
					7.312	-0.0343/-0.044	La2O3	Li2O	Zr4O	LiZr2Os
					8.125	-0.0333	La2O3	Li2O	Zr	LiZr2Os
Li55La24Zr15AsO96	Zr	As	5	-3.138	0.625	-0.0215/-0.034	La2O3	Li2O	Li6Zr2O7	As
					0.750	-0.0264/-0.038	La2O3	Li2O	Li6Zr2O7	LiAs
					1.000	-0.0357/-0.048	La2O3	Li2O	Li6Zr2O7	Li3LaAs2
					2.125	-0.0371/-0.048	La2O3	Li2O	Li6Zr2O7	Zr3As
					7.125	-0.0393/-0.049	La2O3	Li2O	Zr3O	Zr3As
					7.375	-0.0393/-0.048	La2O3	Li2O	Zr4O	Zr3As
					8.125	-0.0382	La2O3	Li2O	Zr	Zr3As
Li55La24Zr15ClO96	Zr	Cl	5	-3.106	0.750	-0.0743/-0.085	La2O3	Li2O	Li6Zr2O7	LiCl
					7.000	-0.0695/-0.078	La2O3	Li2O	Zr3O	LiCl
					7.312	-0.0691/-0.077	La2O3	Li2O	Zr4O	LiCl
					8.250	-0.0669	La2O3	Li2O	Zr	LiCl
Li55La24Zr15IO96	Zr	I	5	-3.119	0.750	-0.0529/-0.064	La2O3	Li2O	Li6Zr2O7	LaIO
					7.000	-0.0524/-0.061	La2O3	Li2O	Zr3O	LaIO
					7.312	-0.0522/-0.061	La2O3	Li2O	Zr4O	LaIO
					8.250	-0.0505	La2O3	Li2O	Zr	LaIO
Li55La24Zr15NbO96	Zr	Nb	5	-3.165	0.250	0.0140/-0.006	La2O3	Li2O	Li6Zr2O7	LiNbO2
					0.625	0.0049/-0.015	La2O3	Li2O	Li6Zr2O7	Nb
					6.875	-0.0064/-0.022	La2O3	Li2O	Zr3O	Nb
					7.187	-0.0067/-0.022	La2O3	Li2O	Zr4O	Nb
					8.125	-0.0063	La2O3	Li2O	Zr	Nb
Li55La24Zr15SbO96	Zr	Sb	5	-3.144	0.625	-0.0156/-0.034	La2O3	Li2O	Li6Zr2O7	Sb
					0.875	-0.0245/-0.043	La2O3	Li2O	Li6Zr2O7	La2SbO2
					1.000	-0.0282/-0.047	La2O3	Li2O	Li6Zr2O7	Li3Sb
					7.250	-0.0327/-0.047	La2O3	Li2O	Zr3O	Li3Sb
					7.562	-0.0327/-0.047	La2O3	Li2O	Zr4O	Li3Sb
					8.500	-0.0316	La2O3	Li2O	Zr	Li3Sb
Li55La24Zr15VO96	Zr	V	5	-3.150	0.250	0.0030/-0.012	La2O3	Li2O	Li6Zr2O7	LiVO2

					0.625	-0.0098/-0.024	La2O3	Li2O	Li6Zr2O7	V
					6.875	-0.0181/-0.029	La2O3	Li2O	Zr3O	V
					7.187	-0.0183/-0.029	La2O3	Li2O	Zr4O	V
					8.125	-0.0175	La2O3	Li2O	Zr	V
Li55La24Zr15TaO96	Zr	Ta	5	-3.172	0.625	0.0117/-0.009	La2O3	Li2O	Li6Zr2O7	Ta
					6.875	-0.0009/-0.017	La2O3	Li2O	Zr3O	Ta
					7.187	-0.0013/-0.017	La2O3	Li2O	Zr4O	Ta
					8.125	-0.0010	La2O3	Li2O	Zr	Ta
Li55La24Zr15PaO96	Zr	Pa	5	-3.179	0.625	0.0186/-0.002	La2O3	Li2O	Li6Zr2O7	Pa
					6.875	0.0045/-0.011	La2O3	Li2O	Zr3O	Pa
					7.187	0.0041/-0.012	La2O3	Li2O	Zr4O	Pa
					8.125	0.0042	La2O3	Li2O	Zr	Pa
Li54La24Zr15TeO96	Zr	Te	6	-3.107	1.000	-0.0836/-0.064	La2O3	Li2O	Li6Zr2O7	La2TeO2
					7.25	-0.0769/-0.061	La2O3	Li2O	Zr3O	La2TeO2
					7.562	-0.0765/-0.061	La2O3	Li2O	Zr4O	La2TeO2
					8.500	-0.0741	La2O3	Li2O	Zr	La2TeO2
Li54La24Zr15MoO96	Zr	Mo	6	-3.118	0.750	-0.0568/-0.041	La2O3	Li2O	Li6Zr2O7	Mo
					1.000	-0.0576/-0.042	La2O3	Li2O	Li6Zr2O7	ZrMo2
					7.042	-0.0562/-0.043	La2O3	Li2O	Zr3O	ZrMo2
					7.344	-0.0560/-0.043	La2O3	Li2O	Zr4O	ZrMo2
					8.250	-0.0543	La2O3	Li2O	Zr	ZrMo2

Table S2. The calculated energy barrier of Li ions migration by BVSE method in ab plane and along c-axis in LLZO and LLZOM, respectively. If ignoring the difference of hopping lengths (a=1Å), and frequencies (ν=10^{13} Hz) in these structures, the estimated diffusion coefficient D will be obtained by the equation $D = \nu a^2 \exp(-E/k_BT)$ at 300K.[2, 3]

System	E_a (eV)	E_b(eV)	E_c(eV)	D_a(cm²/s)	D_b(cm²/s)	D_c(cm²/s)
$Li_7La_3Zr_2O_{12}$	0.94	0.95	0.94	1.62E-19	1.10E-19	1.62E-19
Fe2+(Zr)	1.06	1.05	1.05	1.56E-21	2.29E-21	2.29E-21
Be2+(Zr)	1.04	1.06	1.06	3.38E-21	1.56E-21	1.56E-21
Mg2+(Zr)	1.06	1.05	1.05	1.56E-21	2.29E-21	2.29E-21
Cd2+(Zr)	1.03	1.04	1.04	4.97E-21	3.38E-21	3.38E-21
Eu2+(Zr)	1.23	1.21	1.22	2.17E-24	4.71E-24	3.20E-24
Cu2+(Zr)	1.05	1.07	1.05	2.29E-21	1.06E-21	2.29E-21
Hg2+(Zr)	1.02	1.04	1.03	7.32E-21	3.38E-21	4.97E-21
Ni2+(Zr)	1.05	1.04	1.04	2.29E-21	3.38E-21	3.38E-21
Ca2+(Zr)	1.03	1.04	1.04	4.97E-21	3.38E-21	3.38E-21
Sr2+(Zr)	1	1.04	1.02	1.59E-20	3.38E-21	7.32E-21
Zn2+(Zr)	1.03	1.05	1.09	4.97E-21	2.29E-21	4.88E-22
Mn2+(Zr)	1.05	1.05	1.05	2.29E-21	2.29E-21	2.29E-21

Co2+(Zr)	1.04	1.07	1.04	3.38E-21	1.06E-21	3.38E-21
Cr3+(Zr)	0.93	0.91	0.91	2.38E-19	5.16E-19	5.16E-19
Rh3+(Zr)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
In3+(Zr)	0.94	0.91	0.91	1.62E-19	5.16E-19	5.16E-19
Tl3+(Zr)	0.93	0.92	0.92	2.38E-19	3.50E-19	3.50E-19
Au3+(Zr)	0.94	0.94	0.93	1.62E-19	1.62E-19	2.38E-19
Sc3+(Zr)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
Tm3+(Zr)	0.94	0.93	0.93	1.62E-19	2.38E-19	2.38E-19
Er3+(Zr)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
Ho3+(Zr)	0.94	0.93	0.93	1.62E-19	2.38E-19	2.38E-19
Sm3+(Zr)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
Y3+(Zr)	0.94	0.93	0.93	1.62E-19	2.38E-19	2.38E-19
Dy3+(Zr)	0.94	0.93	0.93	1.62E-19	2.38E-19	2.38E-19
Tb3+(Zr)	0.94	0.93	0.93	1.62E-19	2.38E-19	2.38E-19
Ce3+(Zr)	0.93	0.93	0.94	2.38E-19	2.38E-19	1.62E-19
Nd3+(Zr)	0.93	0.93	0.93	2.38E-19	2.38E-19	2.38E-19
Bi3+(Zr)	0.94	0.93	0.93	1.62E-19	2.38E-19	2.38E-19
Ga3+(Zr)	0.93	0.92	0.92	2.38E-19	3.50E-19	3.50E-19
Al3+(Zr)	0.91	0.91	0.9	5.16E-19	5.16E-19	7.60E-19
Fe3+(Zr)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
Ru3+(Zr)	0.93	0.92	0.92	2.38E-19	3.50E-19	3.50E-19
As3+(Zr)	0.92	0.94	0.92	3.50E-19	1.62E-19	3.50E-19
Co3+(Zr)	0.93	0.92	0.92	2.38E-19	3.50E-19	3.50E-19
P3+(Zr)	0.9	0.91	0.92	7.60E-19	5.16E-19	3.50E-19
Th4+(Zr)	0.93	0.93	0.95	2.38E-19	2.38E-19	1.10E-19
Ce4+(Zr)	0.93	0.93	0.93	2.38E-19	2.38E-19	2.38E-19
C4+(Zr)	0.93	0.93	0.91	2.38E-19	2.38E-19	5.16E-19
Si4+(Zr)	0.93	0.94	0.93	2.38E-19	1.62E-19	2.38E-19
Sn4+(Zr)	0.94	0.94	0.94	1.62E-19	1.62E-19	1.62E-19
Hf4+(Zr)	0.94	0.94	0.94	1.62E-19	1.62E-19	1.62E-19
Ti4+(Zr)	0.94	0.94	0.94	1.62E-19	1.62E-19	1.62E-19
Ge4+(Zr)	0.93	0.94	0.93	2.38E-19	1.62E-19	2.38E-19
Pb4+(Zr)	0.94	0.95	0.93	1.62E-19	1.10E-19	2.38E-19
Mo4+(Zr)	0.92	0.95	0.92	3.50E-19	1.10E-19	3.50E-19
Pt4+(Zr)	0.93	0.95	0.93	2.38E-19	1.10E-19	2.38E-19
Pd4+(Zr)	0.93	0.94	0.93	2.38E-19	1.62E-19	2.38E-19
W4+(Zr)	0.93	0.94	0.93	2.38E-19	1.62E-19	2.38E-19
Se4+(Zr)	0.93	0.96	0.93	2.38E-19	7.46E-20	2.38E-19
Ir4+(Zr)	0.93	0.94	0.93	2.38E-19	1.62E-19	2.38E-19
Te4+(Zr)	0.94	0.94	0.93	1.62E-19	1.62E-19	2.38E-19
Ru4+(Zr)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
Re4+(Zr)	0.93	0.93	0.92	2.38E-19	2.38E-19	3.50E-19
Os4+(Zr)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
S4+(Zr)	0.95	0.95	0.92	1.10E-19	1.10E-19	3.50E-19
Ta5+(Zr)	0.9	0.91	0.9	7.60E-19	5.16E-19	7.60E-19

Nb5+(Zr)	0.91	0.91	0.91	5.16E-19	5.16E-19	5.16E-19
V5+(Zr)	0.9	0.91	0.9	7.60E-19	5.16E-19	7.60E-19
As5+(Zr)	0.91	0.94	0.92	5.16E-19	1.62E-19	3.50E-19
Sb5+(Zr)	0.93	0.92	0.93	2.38E-19	3.50E-19	2.38E-19
I5+(Zr)	0.92	0.89	0.93	3.50E-19	1.12E-18	2.38E-19
Mo6+(Zr)	0.91	0.86	0.89	5.16E-19	3.57E-18	1.12E-18
Te6+(Zr)	0.88	0.88	0.88	1.65E-18	1.65E-18	1.65E-18
W6+(Zr)	0.92	0.93	0.92	3.50E-19	2.38E-19	3.50E-19
Na1+(La)	1.04	1.06	1.06	3.38E-21	1.56E-21	1.56E-21
K1+(La)	1.05	1.06	1.06	2.29E-21	1.56E-21	1.56E-21
Rb1+(La)	1.08	1.06	0.99	7.19E-22	1.56E-21	2.34E-20
Cs1+(La)	1.07	1.07	1.05	1.06E-21	1.06E-21	2.29E-21
Ag1+(La)	1.09	1.1	1.09	4.88E-22	3.32E-22	4.88E-22
Sr2+(La)	1.05	1.05	1.05	2.29E-21	2.29E-21	2.29E-21
Ba2+(La)	1.06	1.04	1.04	1.56E-21	3.38E-21	3.38E-21
Ca2+(La)	1.04	1.03	1.04	3.38E-21	4.97E-21	3.38E-21
Pb2+(La)	1.06	1.04	1.04	1.56E-21	3.38E-21	3.38E-21
Cd2+(La)	1.03	1.05	1.05	4.97E-21	2.29E-21	2.29E-21
Bi3+(La)	0.94	0.92	0.92	1.62E-19	3.50E-19	3.50E-19
Dy3+(La)	0.94	0.94	0.92	1.62E-19	1.62E-19	3.50E-19
Er3+(La)	0.94	0.94	0.93	1.62E-19	1.62E-19	2.38E-19
Ho3+(La)	0.94	0.94	0.93	1.62E-19	1.62E-19	2.38E-19
Lu3+(La)	0.93	0.93	0.92	2.38E-19	2.38E-19	3.50E-19
Nd3+(La)	0.94	0.94	0.91	1.62E-19	1.62E-19	5.16E-19
Pr3+(La)	0.94	0.94	0.92	1.62E-19	1.62E-19	3.50E-19
Sm3+(La)	0.93	0.93	0.91	2.38E-19	2.38E-19	5.16E-19
Tb3+(La)	0.94	0.94	0.92	1.62E-19	1.62E-19	3.50E-19
Y3+(La)	0.93	0.93	0.91	2.38E-19	2.38E-19	5.16E-19
Tm3+(La)	0.94	0.94	0.93	1.62E-19	1.62E-19	2.38E-19
Gd3+(La)	0.94	0.94	0.92	1.62E-19	1.62E-19	3.50E-19
Yb3+(La)	0.94	0.94	0.92	1.62E-19	1.62E-19	3.50E-19
Tl3+(La)	0.95	0.95	0.93	1.10E-19	1.10E-19	2.38E-19
Sc3+(La)	0.96	0.97	0.94	7.46E-20	5.07E-20	1.62E-19
Al3+(Li)	0.92	0.91	0.85	3.50E-19	5.16E-19	5.26E-18
Ga3+(Li)	0.94	0.92	0.87	1.62E-19	3.50E-19	2.42E-18
B3+(Li)	0.95	0.93	0.85	1.10E-19	2.38E-19	5.26E-18
Fe3+(Li)	0.94	0.92	0.85	1.62E-19	3.50E-19	5.26E-18
Cd2+(Li)	0.92	0.89	0.91	3.50E-19	1.12E-18	5.16E-19
Be2+(Li)	0.9	0.9	0.91	7.60E-19	7.60E-19	5.16E-19
Zn2+(Li)	0.9	0.9	0.9	7.60E-19	7.60E-19	7.60E-19
Co2+(Li)	0.92	0.9	0.91	3.50E-19	7.60E-19	5.16E-19
Mn2+(Li)	0.93	0.9	0.9	2.38E-19	7.60E-19	7.60E-19
Cu2+(Li)	0.92	0.9	0.91	3.50E-19	7.60E-19	5.16E-19
Pb4+(Li)	0.9	0.91	0.9	7.60E-19	5.16E-19	7.60E-19
Ti4+(Li)	0.94	0.91	0.95	1.62E-19	5.16E-19	1.10E-19

Table S3. The formation energies of the M_xO_y come from Materials Project Database.[1] The experimental formation energies[4, 5] as a feature is used by machine learning. Most of the formation energies are experimental values, only a few are calculated.

M_xO_y	$\Delta H_{f,x+y}$(eV/atom)		M_xO_y	$\Delta H_{f,x+y}$(eV/atom)		M_xO_y	$\Delta H_{f,x+y}$(eV/atom)	
System	Exp.	Cal.	System	Exp.	Cal.	System	Exp.	Cal.
MgO	-3.118	-3.065	Tb_2O_3	-3.866	-4.002	RuO_2	-1.054	-1.470
CdO	-1.342	-1.382	Tm_2O_3	-3.915	-4.108	TcO_2	-1.496	-1.900
EuO	-3.057	-3.136	Gd_2O_3	-3.813	-3.906	OsO_2	-1.019	-1.361
CuO	-0.807	-0.953	Yb_2O_3	-	-2.721	ReO_2	-1.523	-1.913
HgO	-0.471	-0.647	In_2O_3	-1.913	-2.013	UO_2	-3.748	-3.774
NiO	-1.242	-0.932	Sc_2O_3	-3.956	-3.984	SO_2	-	-1.759
CaO	-3.29	-3.312	Pu_2O_3	-3.462	-3.452	As_2O_3	-1.363	-1.641
MnO	-1.996	-2.000	Al_2O_3	-3.473	-3.442	CO_2	-	-1.783
FeO	-1.415	-1.679	Ga_2O_3	-2.261	-2.281	SO_2	-	-1.759
CoO	-1.233	-1.330	B_2O_3	-2.640	-2.813	Pa_2O_5	-	-2.742
SrO	-3.063	-3.093	Fe_2O_3	-1.71	-1.886	Ta_2O_5	-3.034	-3.355
BaO	-2.840	-2.835	P_2O_3	-	-1.972	Nb_2O_5	-2.812	-3.066
PbO	-1.133	-1.481	N_2O_3	-	-0.607	V_2O_5	-2.296	-2.316
BeO	-3.158	-3.115	Co_2O_3	-	-1.057	As_2O_5	-1.371	-1.576
ZnO	-1.816	-1.797	Am_2O_3	-3.504	-	Sb_2O_5	-1.439	-1.766
Cr_2O_3	-2.364	-2.350	ThO_2	-4.237	-4.387	I_2O_5	-	-0.772
Rh_2O_3	-0.737	-1.087	CeO_2	-3.767	-3.945	Cl_2O_5	-	-0.224
Tl_2O_3	-0.802	-1.120	SiO_2	-3.146	-3.285	Np_2O_5	-3.201	-3.447
Au_2O_3	-0.007	-0.466	SnO_2	-1.996	-2.125	MoO_3	-1.929	-2.023
Ce_2O_3	-3.731	-3.777	HfO_2	-3.854	-4.039	TeO_3	-	-1.359
Ir_2O_3	-	-0.958	TiO_2	-3.261	-3.519	UO_3	-3.171	-3.131
Ru_2O_3	-	-1.141	GeO_2	-2.003	-2.094	WO_3	-2.184	-2.178
Bi_2O_3	-	-1.654	PbO_2	-0.948	-1.317	Na_2O	-1.444	-1.454
Ac_2O_3	-	-3.752	MoO_2	-2.036	-2.150	K_2O	-1.250	-1.257
Dy_2O_3	-3.861	-4.027	PtO_2	-	-0.940	Rb_2O	-1.168	-1.118
Er_2O_3	-3.934	-4.074	PdO_2	-	-0.740	Cs_2O	-1.197	-1.197
Ho_2O_3	-3.899	-4.052	CoO_2	-	-1.138	Ag_2O	-0.108	-0.329
Lu_2O_3	-3.893	-4.139	MnO_2	-1.797	-1.811	Br_2O_3	-	-0.209
Nd_2O_3	-3.748	-3.799	WO_2	-2.038	-2.024	Sm_2O_3	-3.787	-3.879
Pm_2O_3	-3.752	-3.854	SeO_2	-0.779	-1.167	TeO_2	-1.122	-1.509
Pr_2O_3	-3.751	-3.750	IrO_2	-0.862	-1.260	Sb_2O_3	-1.469	-1.767

Table S4. Bond Dissociation Energies of M-O from handbook of Chemical Bond Energies.[6]

M-O	Bond Dissociation Energy(BDE)		M-O	Bond Dissociation Energy(BDE)	
	KJ/mol	eV		KJ/mol	eV
Mg-O	358.2	3.71	Ti-O	666.5	6.91
Cd-O	236	2.45	Ge-O	657.5	6.81
Eu-O	473	4.90	Pb-O	382.4	3.96
Cu-O	287.4	2.98	Mo-O	502	5.20
Hg-O	269	2.79	Pt-O	418.6	4.34
Ni-O	366	3.79	Pd-O	238.1	2.47
Ca-O	383.3	3.97	W-O	720	7.46
Sr-O	426.3	4.42	Se-O	429.7	4.45
Zn-O	250	2.59	Te-O	377	3.91
Mn-O	362	3.75	Tc-O	548	5.68
Co-O	397.4	4.12	Re-O	627	6.50
Cr-O	461	4.78	Os-O	575	5.96
Rh-O	405	4.20	Pa-O	792	8.21
In-O	346	3.59	Ta-O	839	8.70
Tl-O	213	2.21	Nb-O	726.5	7.53
Au-O	223	2.31	V-O	637	6.60
Sc-O	671.4	6.96	As-O	484	5.02
Tm-O	514	5.33	Sb-O	434	4.50
Er-O	606	6.28	I-O	233.4	2.42
Ho-O	606	6.28	Cl-O	267.47	2.77
Y-O	714.1	7.40	Be-O	437	4.53
Dy-O	615	6.37	Nd-O	703	7.29
Tb-O	694	7.19	Sm-O	573	5.94
Ce-O	790	8.19	Na-O	270	2.80
Pm-O	674	6.99	K-O	271.5	2.81
Bi-O	337.2	3.49	Rb-O	276	2.86
Ga-O	374	3.88	Cs-O	293	3.04
Al-O	501.9	5.20	Ag-O	221	2.29
Ir-O	414	4.29	Ba-O	562	5.82
Fe-O	407	4.22	Ac-O	794	8.23
Ru-O	528	5.47	Lu-O	669	6.93
P-O	589	6.10	Pr-O	740	7.67
Th-O	877	9.09	Y-O	714.1	7.40
Sn-O	528	5.47	Yb-O	387.7	4.02
Hf-O	801	8.30	Be-O	437	4.53

Table S5. A summary of top-5 models with two feature pair in the SVM algorithm.[7] For each feature pair, we used five-fold cross-validation on a 0.8/0.2 training/testing split of the dataset. In (score±error), score and error are calculated as the mean score. Accuracy is calculated as the fraction of correctly predicted materials as stable or unstable. Precision is defined as the fraction of predicted stable compounds that are actually stable, and recall is defined as the fraction of actual stable compounds that are predicted stable. The F_1 score is a metric that incorporates both precision and recall.

Feature pair	Accuracy	Precision	Recall	F_1 score
($\Delta H_{f,x+y}$, CN*$\Delta H_{f,x}$)	0.99(±0.02)	0.98(±0.03)	0.99(±0.01)	0.99(±0.02)
($\Delta H_{f,x+y}$, BDE)	0.98(±0.04)	0.97(±0.06)	0.99(±0.02)	0.98(±0.05)
($\Delta H_{f,x+y}$, χ_M)	0.98(±0.02)	0.97(±0.04)	0.99(±0.02)	0.98(±0.03)
($\Delta H_{f,x+y}$, CN*$\Delta H_{f,y}$)	0.97(±0.02)	0.95(±0.04)	0.98(±0.02)	0.96(±0.03)
($\Delta H_{f,x+y}$, 1st IE_M)	0.97(±0.04)	0.95(±0.06)	0.98(±0.03)	0.95(±0.05)

Table S6. Model predicted 18 LLZOM systems with relevant statistics, label 1 and -1 are thermodynamically stable and unstable, respectively. Seven of the systems were verified by DFT calculation.

System	*MxOy*	$\Delta H_{f,x+y}$ (eV/atom)	χ_M	Predicted ΔG (eV/f.u.)	Calculated ΔG (eV/f.u.)	Reaction products
Pm^{3+}(Zr)	Pm_2O_3	-3.752	1.13	0.322	0.183	Li2O3, Li2O, Zr4O, Pm2O3
Pm^{3+}(La)	Pm_2O_3	-3.752	1.13	0.247	0.198	Li2O3, Li2O, Zr4O, Pm2O3
U^{4+}(Zr)	UO_2	-3.748	1.38	0.189	0.020	Li2O3, Li2O, Zr4O, U
Th^{4+}(Zr)	ThO_2	-4.237	1.32	0.250	0.004	Li2O3, Li2O, Zr4O, La2Th8O19
Ac^{3+}(La)	Ac_2O_3	-3.580	1.09	0.169	0.230	Li2O3, Li2O, Zr4O, Ac2O3
Ce^{3+}(La)	Ce_2O_3	-3.731	1.12	0.257	0.155	Li2O3, Li2O, Zr4O, CeO
Sc^{3+}(La)	Sc_2O_3	-3.956	1.36	0.016	-0.008	Li2O3, Li2O, Zr4O, LiScO2
W^{6+}(Zr)	WO_3	-2.184	2.12	-0.456	-0.802	Li2O3, Li2O, Zr4O, ZrW2
As^{3+}(Zr)	As_2O_3	-1.363	2.18	-0.377	-0.725	Li2O3, Li2O, Zr4O, Zr3As
Co^{3+}(Zr)	Co_2O_3	-1.057	1.88	-0.213	-0.626	Li2O3, Li2O, Zr4O, Zr3Co
Pa^{5+}(Zr)	Pa_2O_5	-2.692	1.54	-0.352	0.127	Li2O3, Li2O, Zr4O, Pa
Co^{2+}(Li)	CoO	-1.233	1.88	-0.212	-0.527	Li2O3, Li2O, Zr4O, Zr3Co
Mn^{2+}(Li)	MnO	-1.996	1.55	-0.216	-0.553	Li2O3, Li2O, Zr4O, ZrMn2
Fe^{2+}(Li)	FeO	-1.415	1.83	-0.216	-0.318	Li2O3, Li2O, Zr4O, Zr3Fe

Mg^{2+}(Li)	MgO	-3.118	1.31	-0.232	-0.086	Li2O3, Li2O, Zr4O, Li5Mg
Cu^{2+}(Li)	CuO	-0.807	1.90	-0.212	-0.568	Li2O3, Li2O, Zr4O, Zr2Cu
Pb^{4+}(Li)	PbO_2	-0.948	1.87	-0.265	-0.564	Li2O3, Li2O, Zr4O, Li17Pb4
Ti^{4+}(Li)	TiO_2	-3.261	1.54	-0.215	-0.066	Li2O3, Li2O, Zr4O, ZrTi2O

Table S7. The structures and band gaps for the list of compounds come from the Materials Project.[1]

Material_Id	**Formula**	**Spacegroup**	**Band Gap (eV)**
mp-2605	CaO	Fmm	3.634
mp-1216	YbO	Fmm	3.460
mp-772185	$Li_6Hf_2O_7$	C2/c	4.413
mp-976280	LiBr	$P6_3mc$	4.935
mp-1185319	LiCl	$P6_3mc$	5.928
mp-4547	La_2TeO_2	I4/mmm	2.029
mp-7233	La_2SeO_2	Pm1	2.407
mp-4511	La_2SO_2	Pm1	3.061
mp-30993	LaIO	P4/nmm	3.289
mp-2292	La_2O_3	Ia	3.532
mp-1960	Li_2O	Fmm	4.899
mp-5418	$Li_6Zr_2O_7$	C2/c	3.944

Table S8 Comparison of mean squared error (MSE) and coefficient of determination (R^2) between five regression models for prediction of reaction energy.

Model	**Linear Regression**	**Gradient Boosting**	**Decision tree Regression**	**Kernel Ridge Regression**	**Random Forest**
MSE	0.15	0.10	0.09	0.04	0.06
R^2	0.69	0.80	0.82	0.92	0.90

(a)

Stability of Dopants in $Li_7La_3Zr_2O_{12}$

Li site
La site
Zr site

IA	IIA							VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA
Li	Be (2+)												B (3+)	C (4+)	N (3+)	O	F
Na (1+)	Mg (2+)	IIIB	IVB	VB	VIB	VIIB							Al (3+)	Si (4+)	P (3+)	S (4+)	Cl (5+)
K (1+)	Ca (2+)	Sc (3+)	Ti (4+)	V (5+)	Cr (3+)	Mn (4+)	Fe (3+)	Co (4+)	Ni (2+)	Cu (2+)	Zn (2+)		Ga (3+)	Ge (4+)	As (5+)	Se (4+)	Br (3+)
Rb (1+)	Sr (2+)	Y (3+)	Zr	Nb (5+)	Mo(4+)	Tc (4+)	Ru (4+)	Rh (3+)	Pd (4+)	Ag (1+)	Cd (2+)		In (3+)	Sn (4+)	Sb (5+)	Te (4+)	I (5+)
Cs (1+)	Ba (2+)	La-Lu	Hf (4+)	Ta (5+)	W (4+)	Re(4+)	Os(4+)	Ir (4+)	Pt (4+)	Au (3+)	Hg (2+)		Tl (3+)	Pb (4+)	Bi (3+)	Po	At
Fr	Ra	Ac-Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub						

La-Lu	La	Ce (4+)	Pr (3+)	Nd (3+)	Pm (3+)	Sm (3+)	Eu (2+)	Gd (3+)	Tb (3+)	Dy (3+)	Ho (3+)	Er (3+)	Tm (3+)	Yb(3+)	Lu (3+)
Ac-Lr	Ac (3+)	Th (4+)	Pa (5+)	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

(b)

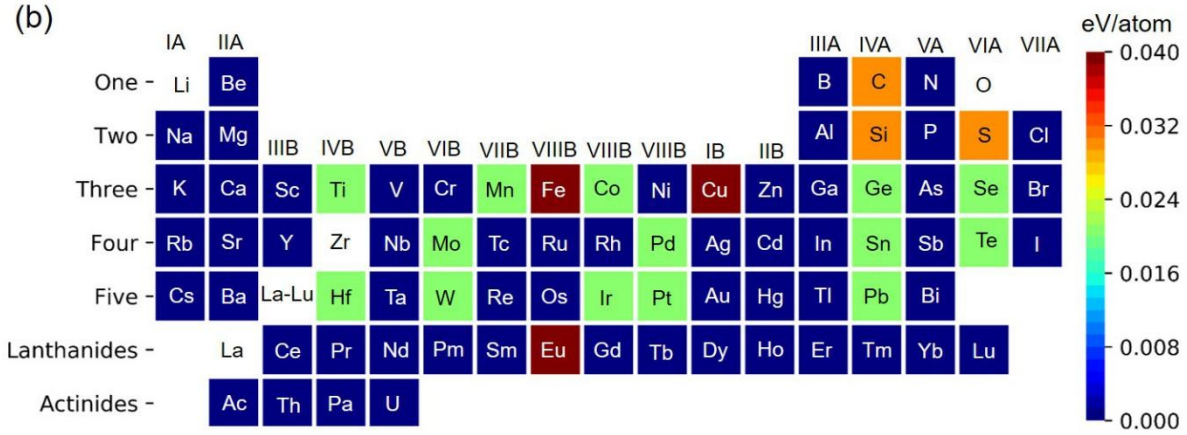

Figure S1. (a) Site and oxidation state preference for the dopant elements in LLZO and (b) calculated their energy above the convex hull.

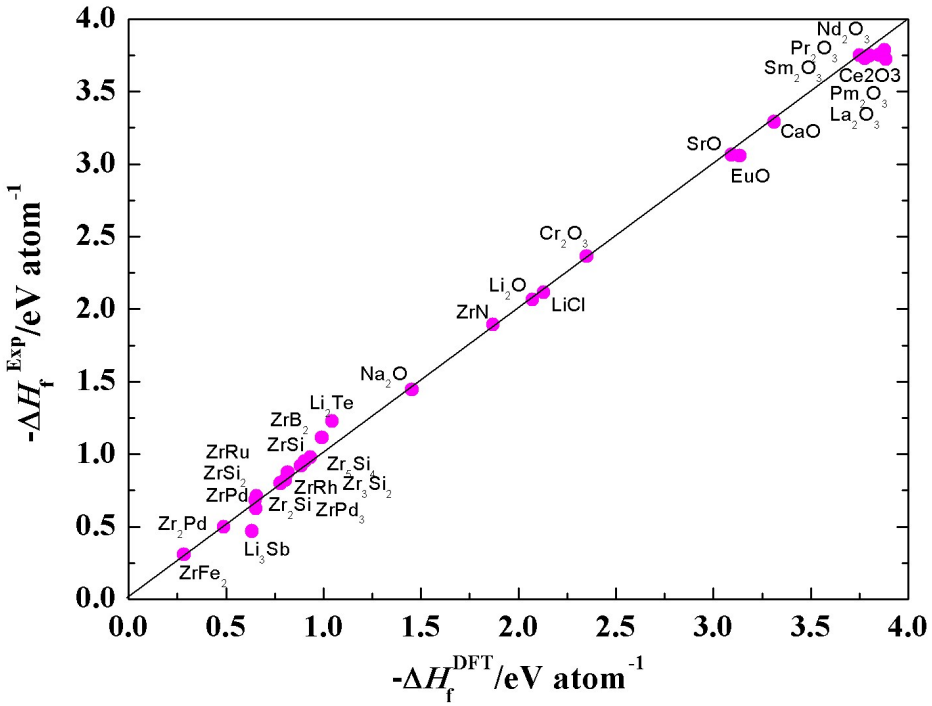

Figure S2. Comparison of the formation energies of some product phases calculated by DFT with the experimental values calculated using available thermodynamic database[4, 5].

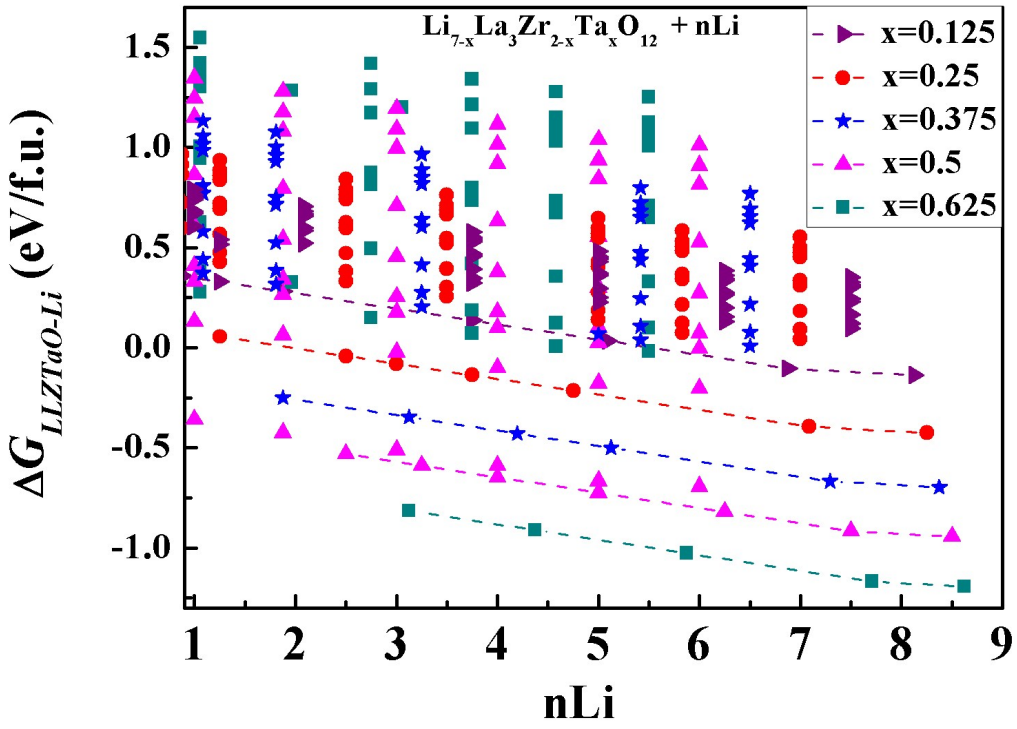

Figure S3. All possible reactions from the automatic reacting screening of $Li_{7-x}La_3Zr_{2-x}Ta_xO_{12}$ (x=0.125, 0.25, 0.375, 0.5, and 0.625) in contacting with different Li concentration (n Li).

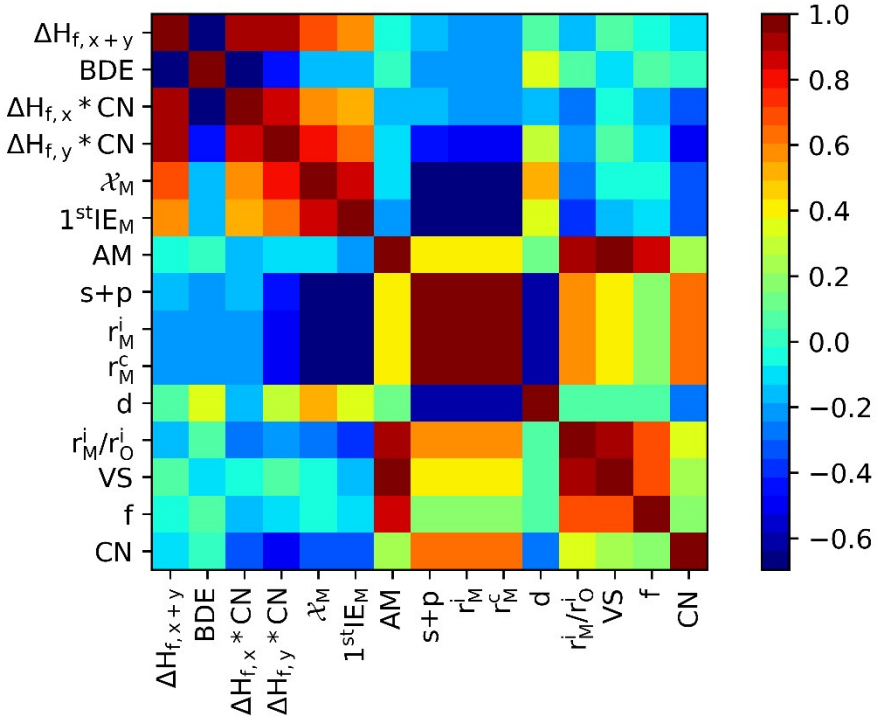

Figure S4. The heat map of Pearson correlation coefficient matrix among the features for LLZOM.

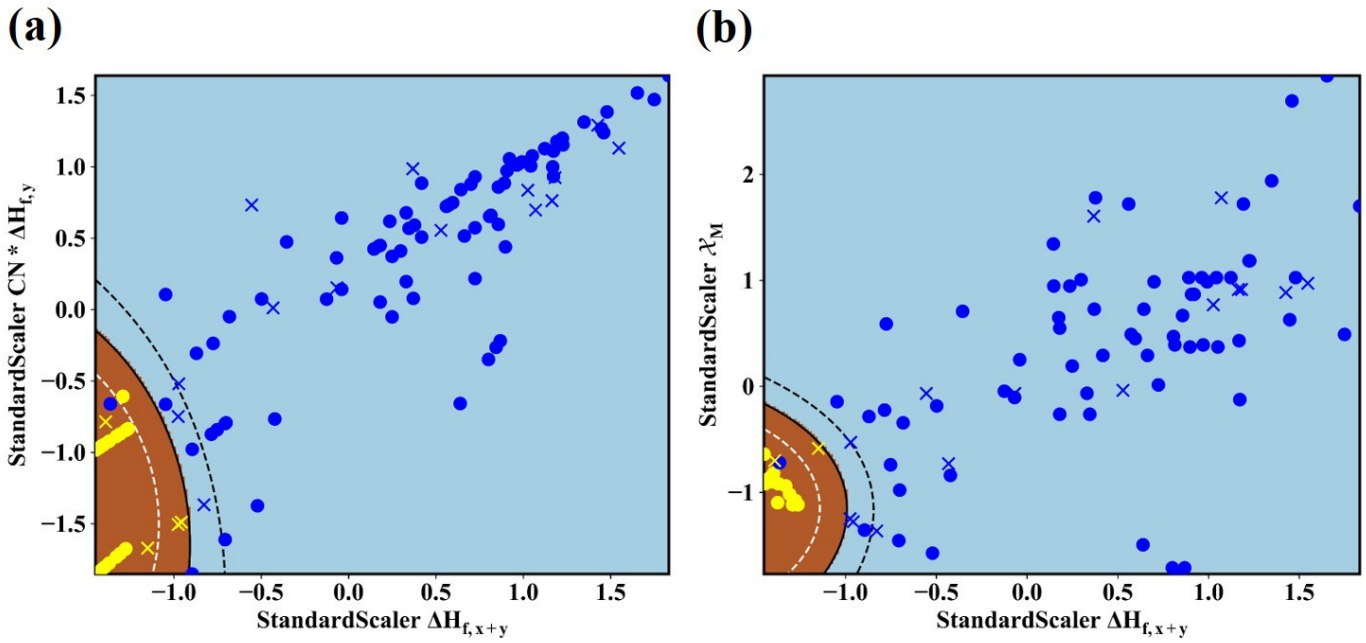

Figure S5. Maps of (a) $\Delta H_{f,x+y}$ and CN*$\Delta H_{f,y}$, (b) $\Delta H_{f,x+y}$ and Pauling electronegativity χ_M feature pairs.

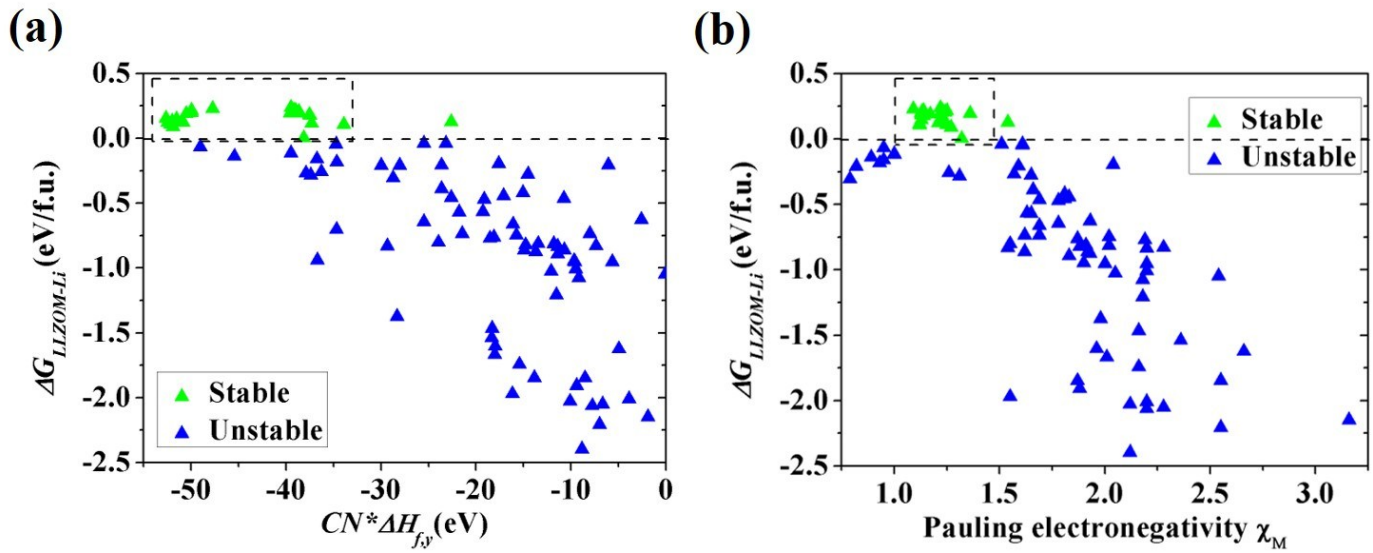

Figure S6. The reaction energy $\Delta G_{LLZOM\text{-}Li}$ of the Li|LLZOM interface dependence on (a) CN*$\Delta H_{f,y}$, and (b) Pauling electronegativity χ_M. The dotted boxes represent the most appropriate ranges for each feature.

References

1. S. P. Ong, W. D. Richards, A. Jain, G. Hautier, M. Kocher, S. Cholia, D. Gunter, V. L. Chevrier, K. A. Persson and G. Ceder, *Computational Materials Science*, 2013, **68**, 314-319.
2. G. H. Vineyard, *Journal of Physics and Chemistry of Solids*, 1957, **3**, 121-127.
3. B. Andriyevsky, K. Doll and T. Jacob, *Materials Chemistry and Physics*, 2017, **185**, 210-217.
4. P. Nash, *https://tptc.iit.edu/index.php/thermo-database*, 2013.

5. *Thermodynamic Properties of Inorganic Materials*, (Springer-Verlag:Berlin, Heidelberg, 1999), **Vol. 19**.
6. Y. R. Luo, *CRC Press, Boca Raton, FL*, 2007.
7. F. Pedregosa, Ga, #235, l. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, #201 and d. Duchesnay, *J. Mach. Learn. Res.*, 2011, **12**, 2825-2830.