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

Strain Effect on Lithium Ions Diffusion in Various Crystal Structures

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Supporting Information

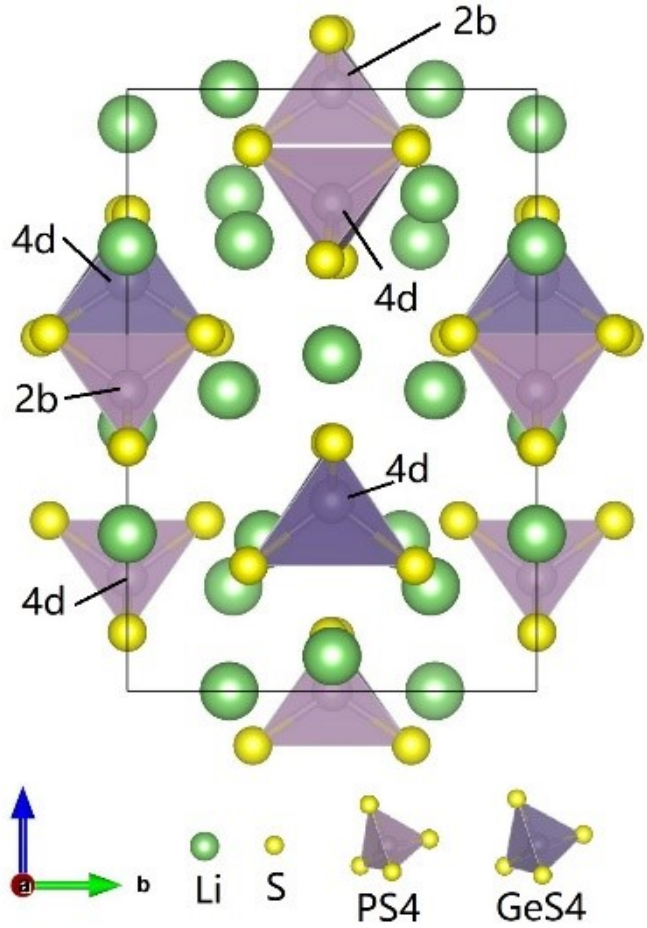

Figure S1. Schematic of the crystal structure of $Li_{10}GeP_2S_{12}$.

Table S1. Comparison of structural parameters of Li_3M, Li_2MN, Li_2MNY_6 and Li_3MY_6 with DFT/Exp values from previous studies, Cal indicates calculated values from our work. All of the structures are face-centered cubic with $\alpha=\beta=\gamma=90°$. Structures of Li_2MNY_6 and Li_3MY_6 are from Materials project, which are theoretical results and waiting for experimental confirmation.

Li_3M index	**Compounds**	**a=b=c (Å)**		**Li_2MN index**	**Compounds**	**a=b=c (Å)**	
		Cal	DFT/Exp			Cal	DFT/Exp
1	Li_3Pd	6.183	6.187[2]	1	Li_2BiAu	6.668	6.670[1]
2	Li_3C	5.280	5.280[1]	2	Li_2AgHg	6.502	6.370[1]
3	Li_3Rh	6.037	5.960[1]	3	Li_2AcTl	7.361	7.300[1]
4	Li_3Mg	6.851	6.860[1]	4	Li_2AgBi	6.746	6.736[4]
5	Li_3Ca	7.489	7.530[1]	5	Li_2CaGe	6.637	6.570[1]
6	Li_3Ga	6.341	6.290[1]	6	Li_2AcAl	7.197	7.200[1]
7	Li_3Pt	6.083	6.010[1]	7	Li_2AgPb	6.682	6.678[4]
8	Li_3Tl	6.684	6.671[2]	8	Li_2AgAu	6.309	6.200[1]
9	Li_3Au	6.305	6.302[2]	9	Li_2CaAl	6.973	6.970[1]
10	Li_3In	6.651	6.590[1]	10	Li_2AgGe	6.265	6.170[1]
11	Li_3Ge	6.228	6.160[1]	11	Li_2CaSi	6.567	6.540[1]
12	Li_3Pb	6.691	6.687[2]	12	Li_2AcIn	7.347	7.330[1]
13	Li_3Bi	6.737	6.708[2]	13	Li_2AgSn	6.540	6.552[4]
14	Li_3Ag	6.456	6.400[1]	14	Li_2AgPd	6.161	6.060[1]
15	Li_3Cd	6.680	6.610[1]	15	Li_2CaTl	7.104	7.020[1]
16	Li_3Sn	6.575	6.572[3]	16	Li_2CaIn	7.085	7.060[1]
17	Li_3Sb	6.562	6.573[2]	17	Li_2CaPb	7.027	6.984[5]
				18	Li_2CaSn	6.936	6.935[5]
				19	Li_2AcPb	7.351	7.290[1]
				20	Li_2AcSn	7.238	7.220[1]

Li_2MNY_6 index	**Compounds**	**a=b=c (Å)**		**Li_3MY_6 index**	**Compounds**	**a=b=c (Å)**	
		Cal	DFT/Exp			Cal	DFT/Exp
1	Li_2AgAsF_6	8.813	8.810[1]	1	Li_3AlF_6	7.522	7.520[1]
2	Li_2AlAgF_6	8.338	8.340[1]	2	Li_3AsF_6	8.030	8.030[1]
3	Li_2AlCuF_6	7.949	7.950[1]	3	Li_3AuF_6	8.156	8.160[1]
4	Li_2AlHgF_6	8.582	8.580[1]	4	Li_3CoF_6	7.580	7.580[1]
5	Li_2CoAgF_6	8.285	8.290[1]	5	Li_3CrF_6	7.724	7.720[1]
6	Li_2CoHgF_6	8.571	8.570[1]	6	Li_3GaF_6	7.703	7.700[1]
7	Li_2CrCuF_6	8.079	8.080[1]	7	Li_3InCl_6	10.039	10.040[1]
8	Li_2CuAsF_6	8.388	8.390[1]	8	Li_3InF_6	8.095	8.090[1]
9	Li_2CuAuF_6	8.406	8.410[1]	9	Li_3IrF_6	7.928	7.930[1]
10	Li_2CuIrF_6	8.246	8.250[1]	10	Li_3MnF_6	7.763	7.760[1]
11	Li_2CuMoF_6	8.394	8.390[1]	11	Li_3MoF_6	8.024	8.020[1]
12	Li_2CuNiF_6	7.909	7.910[1]	12	Li_3NbF_6	8.091	8.090[1]
13	$Li_2CuSbCl_6$	10.215	10.220[1]	13	Li_3NiF_6	7.632	7.630[1]

14	Li_2CuSbF_6	8.661	8.660[1]	14	Li_3PdF_6	7.959	7.960[1]
15	Li_2FeAgF_6	8.357	8.360[1]	15	Li_3RhF_6	7.879	7.880[1]
16	Li_2FeHgF_6	8.781	8.780[1]	16	Li_3RuF_6	7.893	7.890[1]
17	Li_2GaCuF_6	8.111	8.110[1]	17	Li_3SbCl_6	10.281	10.280[1]
18	$Li_2InCuCl_6$	10.018	10.020[1]	18	Li_3SbF_6	8.331	8.330[1]
19	Li_2InCuF_6	8.446	8.450[1]	19	Li_3TaF_6	8.074	8.070[1]
				20	Li_3TiF_6	7.844	7.840[1]
				21	Li_3TlF_6	8.282	8.280[1]
				22	Li_3VF_6	7.772	7.770[1]
				23	Li_3YF_6	8.295	8.300[1]
				24	Li_3ScCl_6	9.921	9.920[1]
				25	Li_3ScF_6	7.944	7.940[1]

Table S2. Comparison of structural parameters of olivine, spinel, layered and lithium super ionic conductor (LISICON) with DFT/Exp values from previous studies, Cal indicates calculated values from our work.

Type	Compounds		a (Å)	b (Å)	c (Å)
Olivine	$LiMnPO_4$	Cal	10.431	6.095	4.737
		DFT/Exp[6]	10.431	6.095	4.737
	$LiFePO_4$	Cal	10.332	6.010	4.692
		DFT/Exp[7]	10.338	6.011	4.695
	$LiCoPO_4$	Cal	10.193	5.917	4.695
		DFT/Exp[8]	10.200	5.920	4.690
	$LiNiPO_4$	Cal	10.028	5.854	4.676
		DFT/Exp[6]	10.028	5.854	4.676
Layered	$LiCoO_2$	Cal	2.843	2.843	14.146
		DFT/Exp[9]	2.816	2.816	14.054
	$LiNiO_2$	Cal	2.905	2.905	14.402
		DFT/Exp[10]	2.891	2.891	14.301
	$LiMnO_2$	Cal	3.022	3.022	14.650
		DFT/Exp[11]	3.005	3.005	14.739
Spinel	$LiMn_2O_4$	Cal	8.422	8.422	8.422
		DFT/Exp[12]	8.433	8.433	8.433
	$LiTi_2O_4$	Cal	8.391	8.391	8.391
		DFT/Exp[13]	8.391	8.391	9.391
	$LiCo_2O_4$	Cal	8.197	8.197	8.197
		DFT/Exp[14]	8.146	8.146	8.146
LISICON	$Li_{10}GeP_2S_{12}$	Cal	8.740	8.740	12.862
		DFT/Exp[15]	8.561	8.847	12.929
	$Li_{10}SnP_2S_{12}$	Cal	8.693	8.969	12.990
		DFT/Exp[15]	8.666	8.950	13.133

$Li_{10}SiP_2S_{12}$	Cal	8.716	8.850	12.716
	DFT/Exp[15]	8.566	8.848	12.920
$Li_{10}GeP_2Se_{12}$	Cal	9.135	9.334	13.500
	DFT/Exp[15]	9.054	9.400	13.690

Table S3. Variation of the energy barriers as a function of the isotropic strains for Li_3M, Li_2MN, Li_2MNY_6, and Li_3MY_6 and the structure corresponding to each color in Figures 6,7,8. The strain variation of Li_2MNY_6 is -7% to 10%.

Type	Compounds	Strain						Color
		-10% (Li_2MNY_6 is -7%)	-5%	0		5%	10%	
				Cal	DFT/ Exp			
Li_3M	Li_3Ag	1.207	0.921	0.696	--	0.519	0.256	Red
	Li_3Au	1.072	0.896	0.534	--	0.381	0.232	OrangeRed
	Li_3Bi	1.370	0.998	0.692	--	0.585	0.512	Brown
	Li_3C	0.747	0.514	0.386	--	0.355	0.310	Yellow
	Li_3Ca	0.702	0.578	0.476	--	0.434	0.193	Olive
	Li_3Ga	0.793	0.646	0.477	--	0.310	0.144	LightGreen
	Li_3Ge	1.166	0.902	0.632	--	0.397	0.053	Green
	Li_3In	0.908	0.765	0.598	--	0.426	0.271	LimeGreen
	Li_3Mg	1.089	0.874	0.467	0.49[16]	0.406	0.324	DarkGreen
	Li_3Pb	1.170	0.924	0.690	--	0.474	0.274	RoyalBlue
	Li_3Pd	0.686	0.523	0.354	--	0.278	0.001	DarkBlue
	Li_3Pt	0.886	0.711	0.484	--	0.389	0.287	Cyan
	Li_3Rh	0.811	0.565	0.410	--	0.247	0.096	Blue
	Li_3Sb	1.526	1.108	0.771	--	0.636	0.570	LightBlue
	Li_3Sn	1.251	1.015	0.761	--	0.510	0.238	Magenta
	Li_3Tl	0.863	0.688	0.516	--	0.359	0.220	Purple
	Li_3Cd	1.162	0.915	0.732		0.520	0.377	DarkRed
Li_2MN	Li_2AcAl	0.972	0.839	0.638	--	0.363	0.020	Red
	Li_2AcIn	1.086	0.949	0.716	--	0.419	0.197	OrangeRed
	Li_2AcPb	1.654	1.321	0.963	--	0.611	0.305	Brown
	Li_2AcSn	1.710	1.390	1.026	--	0.648	0.329	Yellow
	Li_2AcTl	1.016	0.840	0.571	--	0.271	0.126	Olive
	Li_2AgAu	1.791	1.146	0.655	--	0.557	0.166	LightGreen
	Li_2AgBi	1.610	1.042	0.604	--	0.480	0.248	Green
	Li_2AgGe	1.857	1.183	0.673	--	0.565	0.195	LimeGreen
	Li_2AgHg	1.584	1.000	0.566	--	0.484	0.025	DarkGreen
	Li_2AgPb	1.677	1.087	0.648	--	0.500	0.036	RoyalBlue

	Li_2AgPd	1.826	1.240	0.766	--	0.368	0.269	DarkBlue
	Li_2AgSn	1.940	1.260	0.746	--	0.627	0.031	Cyan
	Li_2BiAu	1.728	1.034	0.499	--	0.427	0.212	Blue
	Li_2CaAl	1.370	0.923	0.672	--	0.483	0.200	LightBlue
	Li_2CaGe	1.341	0.912	0.627	--	0.399	0.135	Magenta
	Li_2CaIn	1.250	1.100	0.812	--	0.536	0.325	Purple
	Li_2CaPb	1.544	1.270	0.899	--	0.567	0.319	DarkRed
	Li_2CaSi	1.332	0.894	0.706	--	0.459	0.161	Plum
	Li_2CaSn	1.624	1.332	0.962	--	0.641	0.321	DarkPink
	Li_2CaTl	1.123	0.938	0.803	--	0.413	0.232	Pink
Li_2MNY_6	Li_2AgAsF_6	0.705	0.245	0.377	--	0.574	0.862	Red
	Li_2AlAgF_6	0.302	0.293	0.541	--	0.624	0.761	OrangeRed
	Li_2AlCuF_6	0.491	0.025	0.294	--	0.459	0.754	Brown
	Li_2AlHgF_6	0.668	0.433	0.653	--	0.708	0.769	Yellow
	Li_2CoAgF_6	0.407	0.248	0.516	--	0.569	0.649	Olive
	Li_2CoHgF_6	0.634	0.085	0.427	--	0.520	0.554	LightGreen
	Li_2CrCuF_6	0.533	0.134	0.301	--	0.460	0.628	Green
	Li_2CuAsF_6	0.626	0.293	0.330	--	0.580	0.730	LimeGreen
	Li_2CuAuF_6	0.701	0.042	0.546	--	0.769	0.909	DarkGreen
	Li_2CuIrF_6	0.590	0.235	0.344	--	0.532	0.738	RoyalBlue
	Li_2CuMoF_6	0.622	0.061	0.373	--	0.511	0.806	DarkBlue
	Li_2CuNiF_6	0.445	0.004	0.298	--	0.451	0.656	Cyan
	$Li_2CuSbCl_6$	0.543	0.451	0.656	--	0.763	0.807	Blue
		0.213	0.072	0.213	--	0.474	0.747	LightBlue
	Li_2CuSbF_6	0.413	0.279	0.546	--	0.656	0.843	Magenta
	Li_2FeAgF_6	0.530	0.409	0.602	--	0.723	0.932	Purple
	Li_2FeHgF_6	0.724	0.069	0.321	--	0.507	0.821	DarkRed
	Li_2GaCuF_6	0.356	0.303	0.561	--	0.717	0.954	Plum
	$Li_2InCuCl_6$	0.623	0.280	0.366	--	0.635	0.854	DarkPink
	Li_2InCuF_6							
Li_3MY_6	Li_3AlF_6	0.760	0.183	0.203	--	0.422	0.967	Red
	Li_3AsF_6	0.604	0.016	0.246	--	0.273	0.512	OrangeRed
	Li_3AuF_6	0.463	0.026	0.302	--	0.383	0.508	Brown
	Li_3CoF_6	0.488	0.109	0.143	--	0.285	0.358	Yellow
	Li_3CrF_6	0.341	0.001	0.212	--	0.284	0.420	Olive
	Li_3GaF_6	0.624	0.153	0.273	--	0.488	0.564	LightGreen
	Li_3InCl_6	0.023	0.420	0.669	--	0.781	1.078	Green
	Li_3InF_6	0.806	0.186	0.347	--	0.636	0.733	LimeGreen
	Li_3IrF_6	0.419	0.134	0.297	--	0.367	0.658	DarkGreen
	Li_3MnF_6	0.285	0.017	0.192	--	0.252	0.396	RoyalBlue
	Li_3MoF_6	0.252	0.187	0.335	--	0.352	0.512	DarkBlue
	Li_3NbF_6	0.316	0.132	0.337	--	0.417	0.609	Cyan
	Li_3NiF_6	0.365	0.047	0.163	--	0.261	0.364	Blue
	Li_3PdF_6	0.160	0.111	0.270	--	0.311	0.548	LightBlue

	Li_3RhF_6	0.231	0.087	0.284	--	0.388	0.458	Magenta
	Li_3RuF_6	0.673	0.168	0.314	--	0.380	0.777	Purple
	Li_3SbCl_6	0.263	0.501	0.637	--	0.690	0.844	DarkRed
	Li_3SbF_6	0.525	0.198	0.290	--	0.409	0.530	Pink
	Li_3TaF_6	0.752	0.094	0.193	--	0.248	0.415	LightPurple
	Li_3TiF_6	0.462	0.028	0.221	--	0.306	0.627	DarkPink
	Li_3TlF_6	0.473	0.190	0.275	--	0.648	0.754	Plum
	Li_3VF_6	0.368	0.009	0.214	--	0.273	0.515	Orange
	Li_3YF_6	0.882	0.079	0.439	--	0.716	0.871	DarkCyan
	Li_3ScCl_6	0.245	0.454	0.674	--	0.905	1.135	Black
	Li_3ScF_6	0.515	0.151	0.355	--	0.612	0.752	Gray

Table S4. Variation of the energy barriers as a function of the isotropic strains for Olivine, spinel, layered and LISICON structures. And the energy barrier in the strain-free case are compared with DFT/Exp values from previous studies. The strain variation of spinel is -10% to 10%.

Type	Compounds	Strain					
		-7% (spinel is -10%)	-5%	0		5%	10%
				Cal	DFT/Exp		
Olivine	$LiFePO_4$	0.499	0.431	0.331	0.32[17]	0.245	0.023
	$LiNiPO_4$	0.648	0.534	0.355	0.36[18]	0.253	0.068
	$LiCoPO_4$	0.554	0.449	0.320	0.36[19]	0.237	0.168
	$LiMnPO_4$	0.501	0.419	0.312	0.304[20]	0.249	0.067
Spinel	$LiMn_2O_4$	0.302	0.397	0.418	0.40[14]	0.608	0.870
	$LiTi_2O_4$	0.265	0.305	0.356	0.33[13]	0.365	0.730
	$LiCo_2O_4$	0.247	0.297	0.337	0.30[14]	0.345	0.353
Layered	$LiCoO_2$-ODH	0.907	0.463	0.379	0.39[21]	0.352	0.304
	$LiCoO_2$-TSH	1.124	0.578	0.201	0.19[22]	0.116	0.012
	$LiNiO_2$-ODH	0.806	0.373	0.237	0.59[23]	0.164	0.072
	$LiNiO_2$-TSH	1.030	0.752	0.114	--	0.089	0.047
	$LiMnO_2$-ODH	0.553	0.355	0.317	0.50[24]	0.269	0.169
	$LiMnO_2$-TSH	1.126	0.780	0.191	0.35[24]	0.070	0.007
LISICON	$Li_{10}GeP_2S_{12}$	0.310	0.288	0.227	0.21[15]	0.211	0.074
	$Li_{10}SnP_2S_{12}$	0.346	0.296	0.247	0.24[15]	0.216	0.137
	$Li_{10}SiP_2S_{12}$	0.320	0.273	0.234	0.20[15]	0.186	0.095
	$Li_{10}GeP_2Se_{12}$	0.352	0.315	0.275	0.19[15]	0.236	0.103

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