Supporting Information

3-D Tunnel TiO_2 Crystal Phase as Fast-Charging Lithium Battery Anode from Stochastic Surface Walking based Material Screening

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1. Theoretical Methods and Calculation detail

1.1 Stochastic surface walking (SSW) global Structure Search

The potential energy surface (PES) of Li_nX was explored using a DFT based SSW global structure search (SSW-DFT). The SSW method is capable of surmounting the high barrier on PES and identifying low energy minima (GM). The efficiency of the method for exploring PES has been demonstrated for both aperiodic (molecules,[1] clusters[2-4]) and periodic (surfaces,[5] crystals[1, 6]) systems. The algorithm of the SSW global optimization method can be found in our previous calculations.[7-9] The key SSW parameters utilized are the same with those utilized previously for exploring PES of carbon and boron,[4, 8] i.e. the Gaussian with being 0.6 Å, the number of Gaussian bias potential being 10. The temperature utilized in Metropolis Monte Carlo (MC) is varied from 3000 to 6000 K. The high temperatures are utilized to verify the obtained GM structure since the structure search is less likely to be trapped in local minimum but tends to explore structures with higher energy at higher MC temperature, e.g. 6000 K.

In the SSW search, we firstly start from the bulk crystal structure of X with Li atoms (in a small supercells) being placed randomly in the interstice sites, and utilize the SSW method to explore all the likely phases. Generally, a series of parallel runs (~10 jobs) are performed for the given initial chemical composition (e.g. Li:X=1:1) and more than 300 minima are collected at the first stage. Next, the stable configurations of the first stage are verified and utilized as input for the next cycle of SSW global exploration, which will again collect more than 300 minima. This process is repeated until a certain total number of minima are collected, typically more than 1000 minima obtained for each chemical composition.

1.2 Stochastic surface walking (SSW) global PES exploration using neural network (NN) potential (SSW-NN method)

The Li_nTiO_2 structure at different compositions has been checked in the small ($Li_nTi_4O_8$, n =2,4,8,12) and large ($Li_nTi_{16}O_{32}$, n = 8,16) supercell periodic calculations by recently developed SSW-NN method as implemented in LASP code.[10-11] The NN simulation is at least 3~4 orders of magnitude faster than DFT, while keeping the accuracy in energy and force comparable with those from DFT. The combination of SSW with NN potential thus allows to fast obtain the global PES of more complex materials.[8-9] The SSW-NN method to explore PES can be divided

into three steps: (a) Global dataset generation based on DFT calculations using selected structures from SSW simulation; (b) NN PES fitting and (c) SSW Global optimization using NN PES. These steps are iteratively performed until the NN potential is transferable and robust enough to describe the global PES and more details can be found in our previous work[12].

(i) **Global dataset generation** The global dataset is built iteratively during the self-learning of NN potential. The initial data of the global dataset comes from the DFT-based SSW simulation and all the other data is taken from NN-based SSW PES exploration. In order to cover all the likely compositions of Li_nTiO_2, SSW simulations have been carried out for different structures (including bulk, layer and cluster), compositions and atom number per unit cell.

(ii) **NN PES construction**

The NN potential is generated using the method as introduced in our previous work (also see www.lasphub.com for LASP project).[12-13] To pursue a high accuracy for PES, we have adopted a large set of power-type structure descriptors (PTSDs), which contains 324 descriptors for every element with only power-type structure descriptors, including 132 2-body, 170 3-body, 22 4-body descriptors, and compatibly, the network utilized is also large involving three-hidden layers (324-80-60-60-1 net), equivalent to 103,743 network parameters in total. Min-max scaling is utilized to normalization the training data sets. Hyperbolic tangent activation functions were used for the hidden layers, while a linear transformation was applied to the output layer of all networks. The limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) method is used to minimize the loss function to match DFT energy, force and stress. The final energy and force criterions of the root mean square errors are around 5.9 meV/atom and 0.161 eV/ Å respectively. To demonstrate the accuracy of NN PES, we select 23 Li_nTiO_2 crystal structures to compare the NN results with the DFT calculation results. It has an average energy error of 7.58 meV/atom, which is quite standard for NN potentials and accurate enough for searching the stable structure candidates. The details for the comparison between DFT and NN results can be found in **Table S1**.

Table S1. Benchmark of NN calculations for Li_nTiO_2 systems as compared with DFT results. Listed data include the compositions, total atom number (N_{atom}), DFT energy, NN energy and energy differences between DFT energy and NN energy (E_{diff}, meV/atom).

composition	N_{atom}	DFT-en (eV)	NN-en (eV)	E_{diff} (meV/atom)
$Li_2Ti_4O_8$	14	-113.260	-113.199	-4.343
$Li_2Ti_4O_8$	14	-113.918	-113.692	-16.203
$Li_8Ti_8O_{16}$	32	-455.703	-454.766	-16.729
$Li_8Ti_8O_{16}$	32	-455.710	-454.769	-16.804
$Li_4Ti_4O_8$	16	-119.873	-120.049	10.991
$Li_4Ti_4O_8$	16	-120.209	-120.126	-5.170
$Li_4Ti_4O_8$	16	-120.124	-120.148	1.527
$Li_4Ti_4O_8$	16	-120.247	-120.246	-0.028
$Li_4Ti_4O_8$	16	-120.246	-120.246	-0.008
$Li_8Ti_4O_8$	20	-128.481	-128.465	-1.596
$Li_8Ti_4O_8$	20	-128.417	-128.482	6.364
$Li_8Ti_4O_8$	20	-128.412	-128.543	13.041
$Li_8Ti_4O_8$	20	-127.936	-127.901	-3.501
$Li_{12}Ti_4O_8$	24	-135.353	-133.496	4.821
$Li_{12}Ti_4O_8$	24	-135.909	-136.112	8.447
$Li_{12}Ti_4O_8$	24	-135.940	-136.112	-7.154
$Li_{12}Ti_4O_8$	24	-136.663	-136.006	27.37
$Li_{16}Ti_{16}O_{32}$	64	-479.421	-480.127	11.032
$Li_{16}Ti_{16}O_{32}$	64	-479.520	-480.203	10.666
$Li_{16}Ti_{16}O_{32}$	64	-480.177	-480.466	4.524
$Li_{16}Ti_{16}O_{32}$	64	-480.491	-480.549	0.904
$Li_{16}Ti_{16}O_{32}$	64	-481.010	-480.985	-0.387
$Li_{16}Ti_{16}O_{32}$	64	-481.208	-481.026	-2.841

*Mean error between DFT energy and NN energy is 7.58 meV/atom.

(iii) SSW Global optimization using NN PES

The global minima at the key compositions of Li_nTiO_2 are identified by SSW-NN, where each composition is simulated in the unit cells of 12 ~ 64 atoms and explored to cover more than 10,000 minima on PES. Thus, a large variety of structures ranging from crystalline to amorphous structures have been obtained from SSW-NN simulation. All the low energy structure candidates from SSW-NN exploration are finally verified by plane wave DFT calculations with high accuracy setups.

1.3 DFT calculations

To obtain more accurate energetics, the plane-wave DFT program, Vienna abinitio simulation package VASP[14] was utilized to converge all the important minima (e.g. the most stable minima), which yields the energetic data reported in all figures. In VASP calculations, the electron-ion interaction was represented by the projector augmented wave (PAW)[15-16] and the exchange-correlation functional utilized was GGA-PBE. The plane-wave energy cutoff utilized is 400 eV and the Monkhorst-Pack k-point meshes are (5×5×5). High accuracy calculations with the kinetic energy cutoff 600 eV and the Monkhorst-Pack k-point mesh with (7×7×7) are also utilized to further check the key results.

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2. Structure gallery for Li_xX phases.

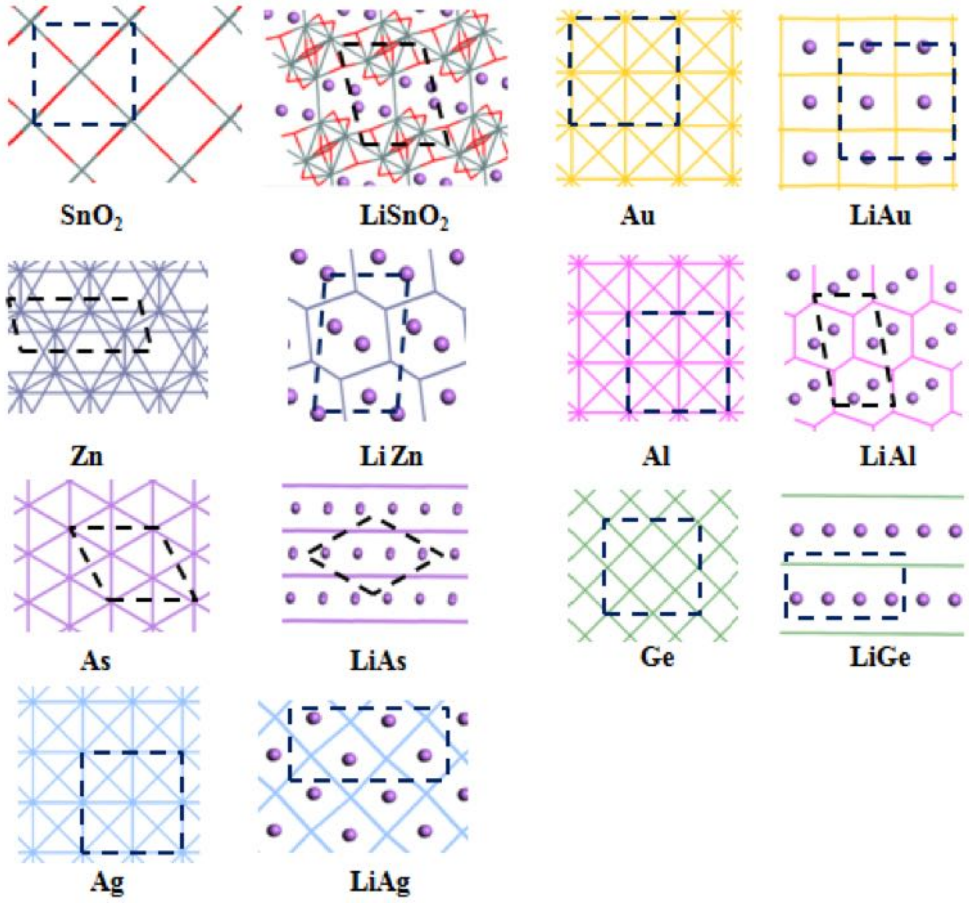

Figure S1 Most stable structures of LiX phases obtained from SSW global search. The initial structure of X is also shown for comparison. Li atoms are represented by magenta balls, while the host X is represented by lines.

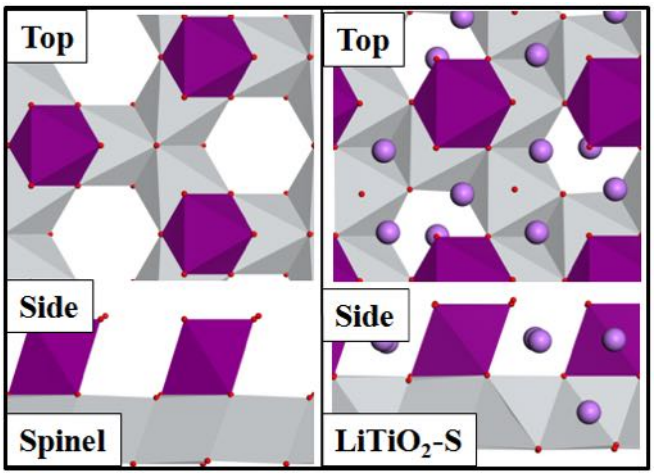

Figure S2 the top and side view of spinel and $LiTiO_2$-S. It in shown that the crystal structure differs from the common spinel structure in that a layer of TiO_6 octahedra per unit cell slips along [100] by half of the lattice length.

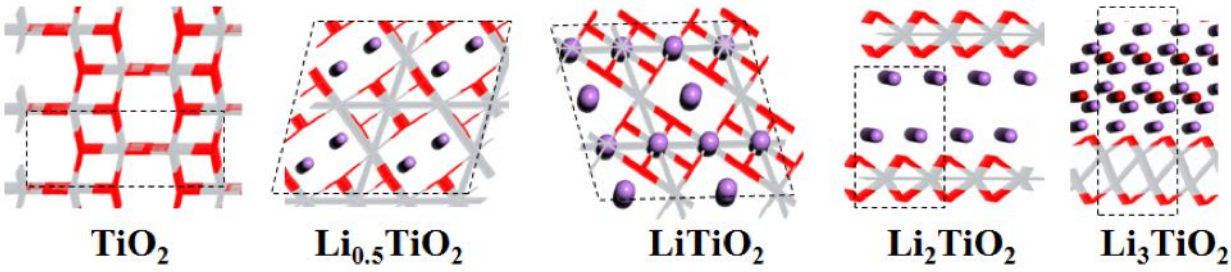

Figure S3 Most stable structures of Li_xTiO_2 obtained from SSW global search. Li atoms are represented by magenta balls, while the host TiO_2 is represented by lines.

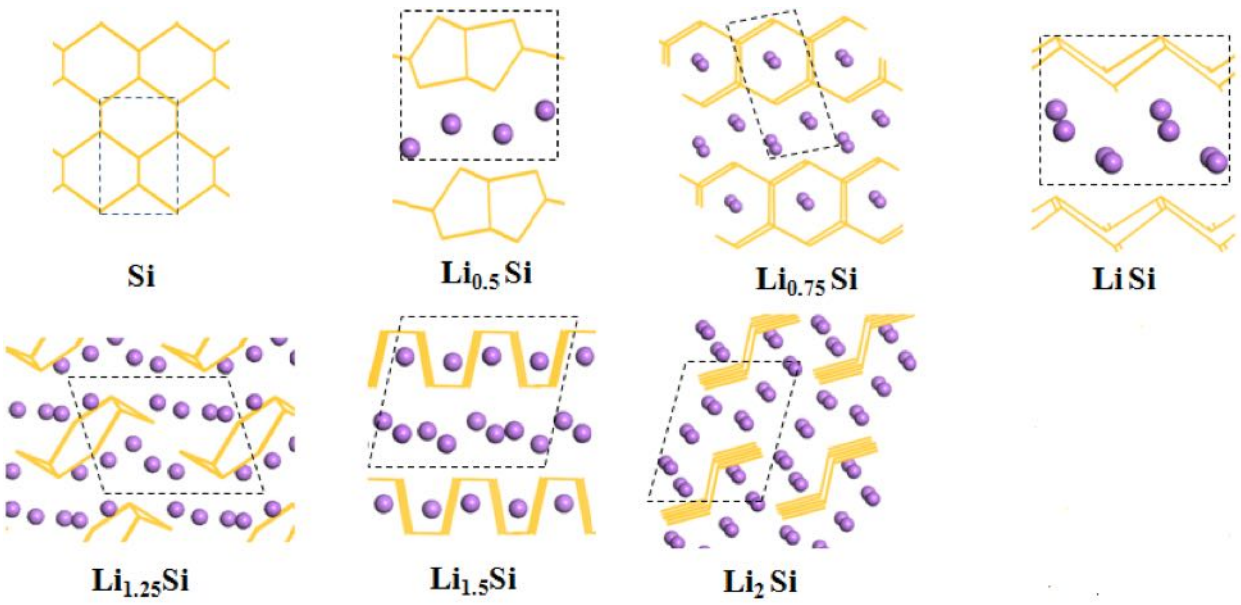

Figure S4 Most stable structures of Li_xSi obtained from SSW global search. Li atoms are represented by magenta balls, while the host Si is represented by lines.

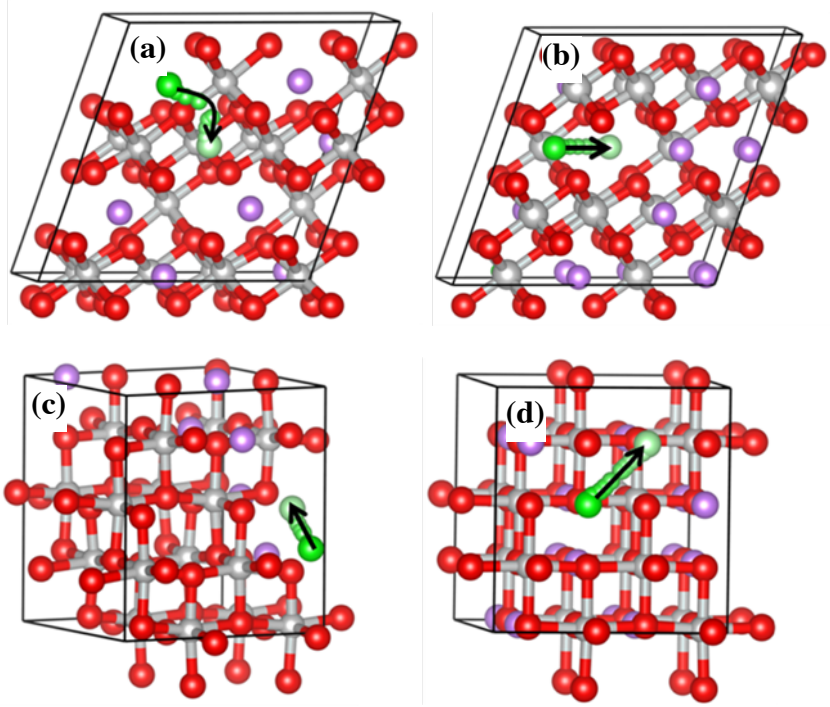

Figure S5 The lowest energy pathway of Li diffusion in (a) $Li_{0.5}TiO_2$-S, (b) $LiTiO_2$-S, (c) $Li_{0.5}TiO_2$-A and (d) $LiTiO_2$-A.

3. The Cartesian coordinates for Li_xX phases obtained from SSW global search

$Li_{0.5}TiO_2$

PBC 10.2628 10.2628 5.9252 89.9998 90.0003 109.4703 (P1)

Li	0.316295444	2.520295259	0.611059977	CORE 1	Li	Li 0.000
Li	5.427157140	6.119004398	3.573695034	CORE 2	Li	Li 0.000
Li	7.158292584	1.310646933	0.658732332	CORE 3	Li	Li 0.000
Li	5.426742055	2.490792029	3.621355486	CORE 4	Li	Li 0.000
Li	-1.415153280	7.328684824	3.621447422	CORE 5	Li	Li 0.000
Li	0.316505645	6.148636232	0.658408972	CORE 6	Li	Li 0.000
Li	3.737522409	7.358318680	0.611150776	CORE 7	Li	Li 0.000
Li	2.006109798	1.281201333	3.573780375	CORE 8	Li	Li 0.000
O	5.300751153	0.639228526	0.625906283	CORE 9	O	O 0.000
O	0.302027941	0.545608229	0.644344218	CORE 10	O	O 0.000
O	2.801690480	7.988704149	2.237051944	CORE 11	O	O 0.000
O	2.940374203	0.650693510	5.199629343	CORE 12	O	O 0.000
O	1.231373660	5.468432737	2.237995302	CORE 13	O	O 0.000
O	0.301025356	8.100109556	0.624020986	CORE 14	O	O 0.000
O	3.581688469	5.482924948	3.607489877	CORE 15	O	O 0.000
O	2.019445945	3.255529909	3.606720322	CORE 16	O	O 0.000
O	2.951875220	0.643805991	1.994437530	CORE 17	O	O 0.000
O	8.063316329	0.638916541	4.957969698	CORE 18	O	O 0.000
O	1.220896105	5.476837933	4.957649542	CORE 19	O	O 0.000
O	6.371675964	5.482471161	1.993963392	CORE 20	O	O 0.000
O	5.439528662	8.094010537	3.606624723	CORE 21	O	O 0.000
O	7.283640739	3.162073488	3.588176539	CORE 22	O	O 0.000
O	0.441267005	8.000346599	3.588306809	CORE 23	O	O 0.000
O	8.073643517	0.631168897	2.238272556	CORE 24	O	O 0.000
O	4.520455305	3.162023084	1.995372120	CORE 25	O	O 0.000
O	5.440725614	0.539573193	3.586715522	CORE 26	O	O 0.000
O	4.510617981	3.170749822	5.200118561	CORE 27	O	O 0.000

O -2.322300168 7.998792666 1.995418121 CORE 28 O O 0.000

O 2.160951631 3.156489083 0.645388038 CORE 29 O O 0.000

O 3.721809867 5.383405593 0.644182224 CORE 30 O O 0.000

O 6.361021051 5.488147783 5.199614054 CORE 31 O O 0.000

O -1.401356797 5.377098809 3.586946763 CORE 32 O O 0.000

O -2.331968204 8.007832137 5.200224423 CORE 33 O O 0.000

O -0.618785050 3.150192936 2.236800054 CORE 34 O O 0.000

O 5.581573689 7.994916571 0.645085253 CORE 35 O O 0.000

O 2.790236208 7.995300000 4.957158518 CORE 36 O O 0.000

O 7.142903368 3.262038757 0.624082142 CORE 37 O O 0.000

O -1.541190023 5.477413486 0.625454565 CORE 38 O O 0.000

O -0.630407914 3.156806928 4.957044906 CORE 39 O O 0.000

O 0.161227631 0.643643984 3.607832484 CORE 40 O O 0.000

Ti 2.874214834 4.317838032 2.119679019 CORE 41 Ti Ti 0.000

Ti 2.868539651 4.321602340 5.082364696 CORE 42 Ti Ti 0.000

Ti 6.295232004 9.155673502 2.119495933 CORE 43 Ti Ti 0.000

Ti 3.727258805 9.154093742 3.597570512 CORE 44 Ti Ti 0.000

Ti 8.854443674 1.900062164 3.597363588 CORE 45 Ti Ti 0.000

Ti 3.730227844 1.901386321 0.634833337 CORE 46 Ti Ti 0.000

Ti 7.151099716 6.739323393 0.634856838 CORE 47 Ti Ti 0.000

Ti 2.012720122 6.737814541 3.597539909 CORE 48 Ti Ti 0.000

Ti 0.306360761 4.316213563 3.597340506 CORE 49 Ti Ti 0.000

Ti 8.000131439 4.321501673 5.075330916 CORE 50 Ti Ti 0.000

Ti 1.163780304 9.155462430 2.112796738 CORE 51 Ti Ti 0.000

Ti 8.005415542 4.317712152 2.112852789 CORE 52 Ti Ti 0.000

Ti 1.158253198 9.159675436 5.075078560 CORE 53 Ti Ti 0.000

Ti -1.405223039 9.161428342 0.635086181 CORE 54 Ti Ti 0.000

Ti 6.289772985 9.159433316 5.082469267 CORE 55 Ti Ti 0.000

Ti 5.436812176 4.323375537 0.634601992 CORE 56 Ti Ti 0.000

$LiTiO_2$-S

PBC 5.87616148 10.18043177 10.10760933 109.08211346 89.99819341 89.99427169

Li	2.480062457	5.371988510	7.462713330	CORE	1 Li Li	0.0000	1
Li	2.479578985	0.281614099	7.462770158	CORE	2 Li Li	0.0000	2
Li	5.298971503	3.642811102	5.000331457	CORE	3 Li Li	0.0000	3
Li	2.601164358	5.294700072	0.222336877	CORE	4 Li Li	0.0000	4
Li	2.598895740	3.663053754	5.149210437	CORE	5 Li Li	0.0000	5
Li	2.360185907	0.204775577	0.224050750	CORE	6 Li Li	0.0000	6
Li	5.295708637	5.315424110	0.375085336	CORE	7 Li Li	0.0000	7
Li	4.031238419	4.474143129	2.691894994	CORE	8 Li Li	0.0000	8
Li	0.927542498	-0.606716317	2.681460570	CORE	9 Li Li	0.0000	9
Li	5.536160029	0.225027939	0.372941051	CORE	10 Li Li	0.0000	10
Li	2.357326448	-1.426994571	5.151004509	CORE	11 Li Li	0.0000	11
Li	3.866425029	2.830672545	7.458149460	CORE	12 Li Li	0.0000	12
Li	5.539007443	-1.447706048	4.998233400	CORE	13 Li Li	0.0000	13
Li	5.417479238	1.933959210	2.686640494	CORE	14 Li Li	0.0000	14
Li	5.417882292	7.024017192	2.686627393	CORE	15 Li Li	0.0000	15
Li	1.092795059	-2.268204376	7.467849257	CORE	16 Li Li	0.0000	16
O	1.087493461	7.749217977	3.892116472	CORE	17 O O	0.0000	17
O	3.929329888	6.242789241	8.647462540	CORE	18 O O	0.0000	18
O	5.430560434	3.619172254	1.497524358	CORE	19 O O	0.0000	19
O	2.465912843	1.967529356	6.273200998	CORE	20 O O	0.0000	20
O	0.990384905	6.153594202	1.501376502	CORE	21 O O	0.0000	21
O	4.024865211	4.645647763	6.257181234	CORE	22 O O	0.0000	22
O	1.086106868	1.207559282	1.481087736	CORE	23 O O	0.0000	23
O	3.928158299	-0.588792480	6.277463689	CORE	24 O O	0.0000	24
O	2.466825524	3.686891139	8.652068328	CORE	25 O O	0.0000	25
O	5.431599773	5.338581550	3.876426386	CORE	26 O O	0.0000	26
O	3.968224996	1.063070540	1.501746736	CORE	27 O O	0.0000	27
O	0.933940803	-0.443365095	6.256921918	CORE	28 O O	0.0000	28
O	2.461177355	8.753762658	1.495018734	CORE	29 O O	0.0000	29

O	5.438045113	7.102243822	6.271624656	CORE	30	O	O	0.0000	30
O	2.499277848	3.664223151	1.495547836	CORE	31	O	O	0.0000	31
O	5.398983057	2.011291408	6.271171547	CORE	32	O	O	0.0000	32
O	2.493098754	7.057222448	6.273578627	CORE	33	O	O	0.0000	33
O	5.404304514	8.709947353	1.497030578	CORE	34	O	O	0.0000	34
O	0.990633671	2.804769972	3.871379194	CORE	35	O	O	0.0000	35
O	4.025298019	1.006823531	8.668234281	CORE	36	O	O	0.0000	36
O	0.935126215	6.098157444	8.668080708	CORE	37	O	O	0.0000	37
O	3.969231117	7.894796143	3.871660598	CORE	38	O	O	0.0000	38
O	1.030850005	1.152349129	8.647770213	CORE	39	O	O	0.0000	39
O	3.872562806	2.660153344	3.891998856	CORE	40	O	O	0.0000	40
O	1.030792142	4.501071566	6.277876736	CORE	41	O	O	0.0000	41
O	3.872299454	6.299086548	1.480841412	CORE	42	O	O	0.0000	42
O	2.459333590	0.203186364	3.877078502	CORE	43	O	O	0.0000	43
O	5.436625792	-1.448476363	8.653787807	CORE	44	O	O	0.0000	44
O	5.398084610	3.641171413	8.653189270	CORE	45	O	O	0.0000	45
O	2.498865056	5.293986452	3.877682031	CORE	46	O	O	0.0000	46
O	2.493153784	-1.403815285	8.652520134	CORE	47	O	O	0.0000	47
O	5.404274391	0.248923380	3.875952401	CORE	48	O	O	0.0000	48
Ti	3.932176663	-0.610762929	2.687649593	CORE	49	Ti	Ti	0.0000	49
Ti	3.964358613	-2.263545674	7.461730905	CORE	50	Ti	Ti	0.0000	50
Ti	1.026580500	4.478844537	2.685684887	CORE	51	Ti	Ti	0.0000	51
Ti	0.994863457	2.827232831	7.463786552	CORE	52	Ti	Ti	0.0000	52
Ti	1.003024659	6.157657221	5.120243804	CORE	53	Ti	Ti	0.0000	53
Ti	3.957694876	7.890488873	0.252553339	CORE	54	Ti	Ti	0.0000	54
Ti	1.019334783	1.148080047	5.028646152	CORE	55	Ti	Ti	0.0000	55
Ti	3.940451383	2.719669649	0.344124601	CORE	56	Ti	Ti	0.0000	56
Ti	2.479947429	7.024072487	2.686488375	CORE	57	Ti	Ti	0.0000	57
Ti	5.417963020	5.371942697	7.462525437	CORE	58	Ti	Ti	0.0000	58

Ti 2.479320702 1.933945639 2.686441982 CORE 59 Ti Ti 0.0000 59

Ti 5.417716953 0.281581303 7.462631827 CORE 60 Ti Ti 0.0000 60

Ti 1.017618009 7.809736880 0.343088102 CORE 61 Ti Ti 0.0000 61

Ti 3.941103743 6.238539203 5.029837227 CORE 62 Ti Ti 0.0000 62

Ti 1.002371260 2.800514165 0.253707428 CORE 63 Ti Ti 0.0000 63

Ti 3.955377088 1.067351634 5.119152814 CORE 64 Ti Ti 0.0000 64

$LiTiO_2$-A

PBC 8.15882320 8.48287302 8.15825322 89.99948143 89.99939061 89.99923249

Ti 2.621893240 4.347227892 3.556537038 CORE 1 Ti Ti 0.0000 1

Ti 6.701300137 4.347234122 3.556555079 CORE 2 Ti Ti 0.0000 2

Ti 2.621935668 4.347782911 7.635460451 CORE 3 Ti Ti 0.0000 3

Ti 6.701355746 4.347786165 7.635441457 CORE 4 Ti Ti 0.0000 4

Ti 0.580518139 6.467028589 3.556360506 CORE 5 Ti Ti 0.0000 5

Ti 4.659919771 6.467037288 3.556330256 CORE 6 Ti Ti 0.0000 6

Ti 2.621793664 2.225943297 1.516262113 CORE 7 Ti Ti 0.0000 7

Ti 6.701164580 2.225944014 1.516250221 CORE 8 Ti Ti 0.0000 8

Ti 0.580360421 0.105925391 1.515920155 CORE 9 Ti Ti 0.0000 9

Ti 4.659747922 0.105927687 1.515926426 CORE 10 Ti Ti 0.0000 10

Ti 0.580411286 0.106332930 5.595201319 CORE 11 Ti Ti 0.0000 11

Ti 4.659836270 0.106337121 5.595195331 CORE 12 Ti Ti 0.0000 12

Ti 0.580555035 6.467841250 7.635652486 CORE 13 Ti Ti 0.0000 13

Ti 4.659980298 6.467849884 7.635682982 CORE 14 Ti Ti 0.0000 14

Ti 2.621831849 2.226343794 5.594899134 CORE 15 Ti Ti 0.0000 15

Ti 6.701265771 2.226346472 5.594910372 CORE 16 Ti Ti 0.0000 16

O 0.582158470 4.352557201 3.556547776 CORE 17 O O 0.0000 17

O 4.661583318 4.352568549 3.556547177 CORE 18 O O 0.0000 18

O 2.620227164 0.111647518 5.595035514 CORE 19 O O 0.0000 19

O 6.699613378 0.111661477 5.595036104 CORE 20 O O 0.0000 20

O	0.582099200	2.220852665	5.594795380	CORE	21	O	O	0.0000	21
O	4.661497481	2.220885845	5.594795500	CORE	22	O	O	0.0000	22
O	0.580229935	0.100311785	7.634723718	CORE	23	O	O	0.0000	23
O	4.659645395	0.100318380	7.634691979	CORE	24	O	O	0.0000	24
O	0.580400953	6.474062976	5.595921959	CORE	25	O	O	0.0000	25
O	4.659813219	6.474027904	5.595926967	CORE	26	O	O	0.0000	26
O	2.621853024	4.340986144	1.516721840	CORE	27	O	O	0.0000	27
O	6.701268658	4.341001104	1.516738473	CORE	28	O	O	0.0000	28
O	2.621847238	2.232777250	7.634832560	CORE	29	O	O	0.0000	29
O	6.701262851	2.232796734	7.634850769	CORE	30	O	O	0.0000	30
O	2.621911788	4.341545085	5.596106975	CORE	31	O	O	0.0000	31
O	6.701329121	4.341529025	5.596089749	CORE	32	O	O	0.0000	32
O	2.621808958	2.231914172	3.555618088	CORE	33	O	O	0.0000	33
O	6.701224566	2.231888074	3.555600649	CORE	34	O	O	0.0000	34
O	2.620351106	6.462465463	7.635660188	CORE	35	O	O	0.0000	35
O	6.699761171	6.462440406	7.635659890	CORE	36	O	O	0.0000	36
O	0.582220775	4.353203662	7.635549484	CORE	37	O	O	0.0000	37
O	4.661619796	4.353197078	7.635550008	CORE	38	O	O	0.0000	38
O	2.620131131	0.111307887	1.515705048	CORE	39	O	O	0.0000	39
O	6.699572490	0.111287061	1.515704019	CORE	40	O	O	0.0000	40
O	0.582017765	2.220545490	1.515945070	CORE	41	O	O	0.0000	41
O	4.661443638	2.220506800	1.515945172	CORE	42	O	O	0.0000	42
O	0.580188450	0.099264049	3.555653668	CORE	43	O	O	0.0000	43
O	4.659600009	0.099252854	3.555686050	CORE	44	O	O	0.0000	44
O	0.580345889	6.473496519	1.516954907	CORE	45	O	O	0.0000	45
O	4.659759302	6.473533604	1.516949880	CORE	46	O	O	0.0000	46
O	2.620297171	6.461784660	3.556397740	CORE	47	O	O	0.0000	47
O	6.699715099	6.461808981	3.556397709	CORE	48	O	O	0.0000	48
Li	2.619454786	0.105617291	7.634151168	CORE	49	Li	Li	0.0000	49

Li	6.698876593	0.105620518	7.634130874	CORE	50	Li	Li	0.0000	50
Li	0.582057967	2.227841510	7.634196926	CORE	51	Li	Li	0.0000	51
Li	4.661490763	2.227844821	7.634236200	CORE	52	Li	Li	0.0000	52
Li	0.582137729	4.345256941	1.516489873	CORE	53	Li	Li	0.0000	53
Li	4.661532852	4.345251183	1.516497360	CORE	54	Li	Li	0.0000	54
Li	0.582176906	4.346111966	5.596015544	CORE	55	Li	Li	0.0000	55
Li	4.661610961	4.346106599	5.596007437	CORE	56	Li	Li	0.0000	56
Li	2.619611573	6.468901462	5.595924457	CORE	57	Li	Li	0.0000	57
Li	6.699068212	6.468898524	5.595945531	CORE	58	Li	Li	0.0000	58
Li	2.619415014	0.103439720	3.554989711	CORE	59	Li	Li	0.0000	59
Li	6.698820849	0.103443641	3.555010024	CORE	60	Li	Li	0.0000	60
Li	0.582076408	2.227404081	3.555053167	CORE	61	Li	Li	0.0000	61
Li	4.661470143	2.227408919	3.555013770	CORE	62	Li	Li	0.0000	62
Li	2.619590331	6.467993855	1.516617032	CORE	63	Li	Li	0.0000	63
Li	6.698966366	6.467988722	1.516595864	CORE	64	Li	Li	0.0000	64

Li_2TiO_2

PBC	5.77065312	4.99793820	8.00766419	81.10829652	97.78396974	89.93679533		
Li	0.420576870	2.851403719	7.597124157	CORE	1	Li	Li	0.0000	1
Li	1.865823552	5.350427768	7.596578053	CORE	2	Li	Li	0.0000	2
Li	0.072418341	4.108868856	4.314838273	CORE	3	Li	Li	0.0000	3
Li	1.512230749	1.609916620	4.314812518	CORE	4	Li	Li	0.0000	4
Li	3.305903431	2.851403719	7.597124157	CORE	5	Li	Li	0.0000	5
Li	-1.019503009	5.350427768	7.596578053	CORE	6	Li	Li	0.0000	6
Li	2.957744902	4.108868856	4.314838273	CORE	7	Li	Li	0.0000	7
Li	4.397557310	1.609916620	4.314812518	CORE	8	Li	Li	0.0000	8
O	0.069653546	0.780098362	3.334444114	CORE	9	O	O	0.0000	9
O	1.515108504	3.279069424	3.334464466	CORE	10	O	O	0.0000	10
O	1.511198955	3.279434592	0.740227164	CORE	11	O	O	0.0000	11

O 0.065846463 0.780405324 0.740213788 CORE 12 O O 0.0000 12

O 2.954980107 0.780098362 3.334444114 CORE 13 O O 0.0000 13

O 4.400435065 3.279069424 3.334464466 CORE 14 O O 0.0000 14

O 4.396525516 3.279434592 0.740227164 CORE 15 O O 0.0000 15

O 2.951173024 0.780405324 0.740213788 CORE 16 O O 0.0000 16

Ti 0.070425921 2.446914467 2.036949050 CORE 17 Ti Ti 0.0000 17

Ti 1.515843504 4.945924424 2.036937948 CORE 18 Ti Ti 0.0000 18

Ti 2.955752482 2.446914467 2.036949050 CORE 19 Ti Ti 0.0000 19

Ti 4.401170065 4.945924424 2.036937948 CORE 20 Ti Ti 0.0000 20

Li_3TiO_3

PBC 3.09280429 5.35851928 12.97816720 89.98340058 90.00222907 90.00893612

Li 1.158025840 5.137471398 5.212470710 CORE 1 Li Li 0.0000 1

Li 1.158468412 5.137674206 9.328442369 CORE 2 Li Li 0.0000 2

Li 2.705639639 0.669619435 7.975753278 CORE 3 Li Li 0.0000 3

Li 1.159836423 1.562038307 6.605003709 CORE 4 Li Li 0.0000 4

Li 2.704670361 0.675160590 12.092005649 CORE 5 Li Li 0.0000 5

Li 2.706590273 2.458234428 5.212465636 CORE 6 Li Li 0.0000 6

Li 1.159596505 3.354341372 12.092150928 CORE 7 Li Li 0.0000 7

Li 2.705587451 2.458447023 9.328421926 CORE 8 Li Li 0.0000 8

Li 1.159120240 3.348869928 7.975690129 CORE 9 Li Li 0.0000 9

Li 2.705507713 4.245822264 10.699840989 CORE 10 Li Li 0.0000 10

Li 2.704899055 4.241318626 6.604993451 CORE 11 Li Li 0.0000 11

Li 1.158583315 1.566586649 10.699817997 CORE 12 Li Li 0.0000 12

O 2.705804050 2.455260229 7.285096006 CORE 13 O O 0.0000 13

O 1.159063720 3.352397288 10.019165089 CORE 14 O O 0.0000 14

O 1.158531811 5.134528075 7.285122685 CORE 15 O O 0.0000 15

O 1.160014942 1.564835494 4.568481536 CORE 16 O O 0.0000 16

O 1.158446572 1.568366853 12.735397197 CORE 17 O O 0.0000 17

O 2.705338803 4.247876970 12.735453351 CORE 18 O O 0.0000 18

O 2.705412680 0.673132100 10.019166073 CORE 19 O O 0.0000 19

O 2.705091414 4.244253990 4.568516713 CORE 20 O O 0.0000 20

Ti 2.705394164 0.672997808 3.212291612 CORE 21 Ti Ti 0.0000 21

Ti 1.159831034 3.352202017 3.212236413 CORE 22 Ti Ti 0.0000 22

Ti 1.158301603 5.135627361 1.113169594 CORE 23 Ti Ti 0.0000 23

Ti 2.706374965 2.456325797 1.113180045 CORE 24 Ti Ti 0.0000 24

$Li_{0.8}Si$

PBC 3.7614 7.9464 7.6757 98.6073 75.9917 89.8451 (P1)

Li1 3.003110000 1.320730000 0.602550000 XXXX 1 xx Li 0.000

Li2 4.902690000 3.484650000 7.277660000 XXXX 1 xx Li 0.000

Li3 1.153120000 3.360420000 1.798550000 XXXX 1 xx Li 0.000

Li4 1.166210000 6.717270000 1.093380000 XXXX 1 xx Li 0.000

Si5 4.915530000 5.986950000 6.301340000 XXXX 1 xx Si 0.000

Si6 3.040940000 5.071290000 2.886260000 XXXX 1 xx Si 0.000

Si7 3.015470000 -0.606620000 5.719900000 XXXX 1 xx Si 0.000

Si8 1.155820000 4.595880000 4.301380000 XXXX 1 xx Si 0.000

Si9 4.912660000 2.239930000 4.783990000 XXXX 1 xx Si 0.000

Si10 3.036090000 1.758540000 6.188830000 XXXX 1 xx Si 0.000

Si11 1.141370000 0.854150000 2.784400000 XXXX 1 xx Si 0.000

Si12 3.020800000 -0.509140000 3.349440000 XXXX 1 xx Si 0.000

$Li_{0.75}Si$

PBC 5.5171 9.4569 4.4124 102.7704 89.7922 106.2977 (P1)

Li1 0.981170000 0.881300000 3.464300000 XXXX 1 xx Li 0.000

Li2 3.744240000 1.018390000 3.488060000 XXXX 1 xx Li 0.000

Li3 0.893870000 -0.069520000 0.969810000 XXXX 1 xx Li 0.000

Li4 0.987180000 5.005650000 2.241810000 XXXX 1 xx Li 0.000

Li5 3.658440000 0.265930000 1.043070000 XXXX 1 xx Li 0.000

Li6 3.748010000 5.169060000 2.260040000 XXXX 1 xx Li 0.000

Si7 2.523500000 3.343190000 4.071900000 XXXX 1 xx Si 0.000

Si8 2.230150000 6.795190000 0.412140000 XXXX 1 xx Si 0.000

Si9 -0.248910000 7.537500000 2.877980000 XXXX 1 xx Si 0.000

Si10 -0.246130000 6.791020000 0.415430000 XXXX 1 xx Si 0.000

Si11 -0.548450000 3.345130000 4.076270000 XXXX 1 xx Si 0.000

Si12 2.272070000 7.532530000 2.876260000 XXXX 1 xx Si 0.000

Si13 2.193480000 2.634750000 1.628280000 XXXX 1 xx Si 0.000

Si14 -0.254950000 2.637600000 1.620710000 XXXX 1 xx Si 0.000

LiSi

PBC 11.6595 3.8092 6.3013 89.6354 105.3310 90.6080 (P1)

Li 1.248723624 2.639560796 1.042954802 CORE 1 Li Li 0.000

Li 7.478535445 0.787157719 6.057124123 CORE 2 Li Li 0.000

Li 8.591429310 0.818282100 3.039220487 CORE 3 Li Li 0.000

Li 2.762176101 0.817693713 3.037453741 CORE 4 Li Li 0.000

Li 7.078747736 2.641489350 1.042795446 CORE 5 Li Li 0.000

Li 0.697756731 2.692900605 4.107115526 CORE 6 Li Li 0.000

Li 6.528758526 2.694195514 4.105968548 CORE 7 Li Li 0.000

Li 1.649492754 0.786309204 6.055041700 CORE 8 Li Li 0.000

Si 9.175298752 2.686358926 5.193800036 CORE 9 Si Si 0.000

Si -1.001282183 0.791955644 4.970452692 CORE 10 Si Si 0.000

Si -0.317617777 0.779097933 2.517976063 CORE 11 Si Si 0.000

Si 5.513382104 0.779898666 2.514831424 CORE 12 Si Si 0.000

Si 4.829083747 0.791838825 4.967344450 CORE 13 Si Si 0.000

Si 3.346911733 2.687018658 5.191293180 CORE 14 Si Si 0.000

Si 4.330771139 2.679021332 1.567947521 CORE 15 Si Si 0.000

Si 10.159635076 2.678567306 1.571032076 CORE 16 Si Si 0.000

$Li_{1.25}Si$

PBC 8.5706 7.5964 5.3794 99.9608 91.9010 110.9751 (P1)

Li1	-0.146480000	3.671360000	0.215270000	XXXX 1	xx	Li	0.000
Li2	0.786980000	-0.049240000	3.495010000	XXXX 1	xx	Li	0.000
Li3	5.746230000	4.682530000	4.647120000	XXXX 1	xx	Li	0.000
Li4	6.844290000	2.027980000	2.657020000	XXXX 1	xx	Li	0.000
Li5	4.099730000	6.269050000	2.225490000	XXXX 1	xx	Li	0.000
Li6	4.286050000	-0.022730000	3.447530000	XXXX 1	xx	Li	0.000
Li7	2.625620000	2.638070000	0.151610000	XXXX 1	xx	Li	0.000
Li8	-0.120030000	6.519420000	0.658160000	XXXX 1	xx	Li	0.000
Li9	2.229810000	4.694570000	4.697010000	XXXX 1	xx	Li	0.000
Li10	4.072350000	3.084870000	2.708670000	XXXX 1	xx	Li	0.000
Si11	1.867880000	4.675880000	1.897720000	XXXX 1	xx	Si	0.000
Si12	6.262550000	4.701720000	1.934610000	XXXX 1	xx	Si	0.000
Si13	1.180360000	2.498600000	2.773010000	XXXX 1	xx	Si	0.000
Si14	4.824100000	1.028810000	0.972850000	XXXX 1	xx	Si	0.000
Si15	0.450100000	1.000560000	0.936650000	XXXX 1	xx	Si	0.000
Si16	6.748690000	0.107970000	4.972340000	XXXX 1	xx	Si	0.000
Si17	-0.225630000	4.514670000	3.183730000	XXXX 1	xx	Si	0.000
Si18	5.522500000	3.203380000	0.095080000	XXXX 1	xx	Si	0.000

$Li_{1.5}Si$

PBC 6.7448 7.9462 7.7971 107.9265 90.9181 113.9558 (P1)

Li1	0.472650000	-0.720800000	3.417000000	XXXX 1	xx	Li	0.000
Li2	-0.629340000	1.459830000	1.605490000	XXXX 1	xx	Li	0.000
Li3	-1.193950000	1.568760000	7.084100000	XXXX 1	xx	Li	0.000
Li4	-1.832110000	6.915840000	0.724870000	XXXX 1	xx	Li	0.000
Li5	-1.385720000	4.117930000	2.587010000	XXXX 1	xx	Li	0.000
Li6	1.747470000	4.211330000	3.949520000	XXXX 1	xx	Li	0.000

Li7 2.413170000 1.477640000 5.704730000 XXXX 1 xx Li 0.000

Li8 3.418300000 1.922230000 0.292360000 XXXX 1 xx Li 0.000

Li9 0.165140000 -0.856960000 6.235090000 XXXX 1 xx Li 0.000

Li10 -0.284030000 1.937990000 4.384980000 XXXX 1 xx Li 0.000

Li11 0.864800000 6.445140000 2.031370000 XXXX 1 xx Li 0.000

Li12 -2.303470000 3.734840000 5.274040000 XXXX 1 xx Li 0.000

Si13 0.123880000 3.868440000 6.293740000 XXXX 1 xx Si 0.000

Si14 3.088340000 4.901570000 1.108460000 XXXX 1 xx Si 0.000

Si15 4.026010000 1.790450000 3.364480000 XXXX 1 xx Si 0.000

Si16 4.635280000 -0.072130000 4.767620000 XXXX 1 xx Si 0.000

Si17 2.353530000 4.081330000 7.024350000 XXXX 1 xx Si 0.000

Si18 1.792610000 1.587980000 2.633620000 XXXX 1 xx Si 0.000

Si19 1.188870000 3.459620000 1.228320000 XXXX 1 xx Si 0.000

Si20 2.735510000 -1.519960000 4.900130000 XXXX 1 xx Si 0.000

Li_3Si

PBC 7.8531 9.3497 6.8031 111.0605 112.4303 71.7114 (P1)

Li1 5.008180000 3.118890000 3.813860000 XXXX 1 xx Li 0.000

Li2 8.957080000 4.397870000 0.420790000 XXXX 1 xx Li 0.000

Li3 7.488820000 -0.055140000 0.428160000 XXXX 1 xx Li 0.000

Li4 2.633480000 1.443170000 4.715240000 XXXX 1 xx Li 0.000

Li5 0.150440000 -0.265870000 5.489980000 XXXX 1 xx Li 0.000

Li6 6.466040000 2.719340000 1.209670000 XXXX 1 xx Li 0.000

Li7 4.084590000 5.829970000 4.716990000 XXXX 1 xx Li 0.000

Li8 2.832210000 6.289780000 1.691600000 XXXX 1 xx Li 0.000

Li9 1.356340000 6.725400000 4.216640000 XXXX 1 xx Li 0.000

Li10 1.590700000 4.186530000 5.487530000 XXXX 1 xx Li 0.000

Li11 4.077160000 0.998010000 2.085510000 XXXX 1 xx Li 0.000

Li12 7.934450000 7.156510000 1.230240000 XXXX 1 xx Li 0.000

Li13 6.432380000 7.582270000 3.857600000 XXXX 1 xx Li 0.000

Li14 -0.095000000 2.267050000 4.222130000 XXXX 1 xx Li 0.000

Li15 1.349700000 1.866880000 1.669700000 XXXX 1 xx Li 0.000

Li16 5.569950000 5.440970000 2.092740000 XXXX 1 xx Li 0.000

Si17 5.328670000 0.563170000 4.900530000 XXXX 1 xx Si 0.000

Si18 8.025740000 4.629480000 2.852300000 XXXX 1 xx Si 0.000

Si19 2.518320000 3.924630000 3.060850000 XXXX 1 xx Si 0.000

Si20 6.538650000 0.237600000 2.850520000 XXXX 1 xx Si 0.000

Si21 3.747190000 3.561400000 1.020210000 XXXX 1 xx Si 0.000

Si22 1.031450000 -0.488840000 3.052670000 XXXX 1 xx Si 0.000

Si23 6.799580000 5.003900000 4.891260000 XXXX 1 xx Si 0.000

Si24 5.207030000 7.997620000 1.023440000 XXXX 1 xx Si 0.000

LiC

PBC 3.8049 5.0341 11.3640 89.6747 89.7633 90.0078 (P1)

Li 2.901961284 4.354943943 2.711896605 CORE 1 Li Li 0.000

Li 1.035872967 1.829337894 2.621036920 CORE 2 Li Li 0.000

Li 1.075406909 1.774641146 8.281736726 CORE 3 Li Li 0.000

Li 2.928648523 4.360815145 11.161727908 CORE 4 Li Li 0.000

Li 2.986998004 4.309049696 5.436143301 CORE 5 Li Li 0.000

Li 3.004177745 4.328049939 8.355424258 CORE 6 Li Li 0.000

Li 1.060667923 1.768128827 5.520119288 CORE 7 Li Li 0.000

Li 1.035840327 1.857234844 11.231305054 CORE 8 Li Li 0.000

C 2.962676925 1.184618059 9.726784769 CORE 9 C C 0.000

C 2.944580260 1.173170119 4.100261758 CORE 10 C C 0.000

C 1.005451739 3.707574557 1.235120035 CORE 11 C C 0.000

C 1.087325468 4.922486926 6.894976263 CORE 12 C C 0.000

C 2.951192266 2.463507597 9.788377786 CORE 13 C C 0.000

C 2.945450230 2.451015112 4.043463056 CORE 14 C C 0.000

C 1.001389810 4.986631484 1.268789304 CORE 15 C C 0.000

C 1.083866039 3.642695231 6.881241965 CORE 16 C C 0.000

LiSn

PBC 6.3181 8.4437 6.3108 89.9049 90.0379 90.0033 (P1)

Li 1.288532298 6.653999897 6.148836204 CORE 1 Li Li 0.000

Li 4.449659152 6.648765029 2.993416757 CORE 2 Li Li 0.000

Li 4.447816683 2.432170572 6.148836459 CORE 3 Li Li 0.000

Li 1.290865523 2.426935732 2.993417117 CORE 4 Li Li 0.000

Li 1.288776582 2.432170498 6.148836168 CORE 5 Li Li 0.000

Li 4.449903366 2.426935757 2.993416758 CORE 6 Li Li 0.000

Li 4.447572440 6.653999911 6.148836517 CORE 7 Li Li 0.000

Li 1.290621272 6.648765084 2.993417093 CORE 8 Li Li 0.000

Sn 2.870822970 0.313429243 1.415844633 CORE 9 Sn Sn 0.000

Sn 6.027774072 0.318664074 4.571264093 CORE 10 Sn Sn 0.000

Sn 2.868735226 0.318664003 4.571264377 CORE 11 Sn Sn 0.000

Sn 6.029861981 0.313429270 1.415845078 CORE 12 Sn Sn 0.000

Sn 2.870578673 4.535258537 1.415844690 CORE 13 Sn Sn 0.000

Sn 6.027529808 4.540493381 4.571264128 CORE 14 Sn Sn 0.000

Sn 6.029617791 4.535258560 1.415844982 CORE 15 Sn Sn 0.000

Sn 2.868491024 4.540493345 4.571264412 CORE 16 Sn Sn 0.000

$LiSnO_2$

PBC 6.3181 8.4437 6.3108 89.9049 90.0379 90.0033 (P1)

Li 1.288532298 6.653999897 6.148836204 CORE 1 Li Li 0.000

Li 4.449659152 6.648765029 2.993416757 CORE 2 Li Li 0.000

Li 4.447816683 2.432170572 6.148836459 CORE 3 Li Li 0.000

Li 1.290865523 2.426935732 2.993417117 CORE 4 Li Li 0.000

Li 1.288776582 2.432170498 6.148836168 CORE 5 Li Li 0.000

Li 4.449903366 2.426935757 2.993416758 CORE 6 Li Li 0.000

Li 4.447572440 6.653999911 6.148836517 CORE 7 Li Li 0.000

Li 1.290621272 6.648765084 2.993417093 CORE 8 Li Li 0.000

Sn 2.870822970 0.313429243 1.415844633 CORE 9 Sn Sn 0.000

Sn 6.027774072 0.318664074 4.571264093 CORE 10 Sn Sn 0.000

Sn 2.868735226 0.318664003 4.571264377 CORE 11 Sn Sn 0.000

Sn 6.029861981 0.313429270 1.415845078 CORE 12 Sn Sn 0.000

Sn 2.870578673 4.535258537 1.415844690 CORE 13 Sn Sn 0.000

Sn 6.027529808 4.540493381 4.571264128 CORE 14 Sn Sn 0.000

Sn 6.029617791 4.535258560 1.415844982 CORE 15 Sn Sn 0.000

Sn 2.868491024 4.540493345 4.571264412 CORE 16 Sn Sn 0.000

LiAu

PBC 6.6727 6.4766 3.0863 89.6263 90.0444 90.1678 (P1)

Li1 4.875740000 3.189060000 1.484970000 XXXX 1 xx Li 0.000

Li2 1.645670000 0.032850000 1.484230000 XXXX 1 xx Li 0.000

Li3 1.609750000 3.162730000 1.488700000 XXXX 1 xx Li 0.000

Li4 4.857030000 6.322930000 1.467260000 XXXX 1 xx Li 0.000

Au5 3.232640000 4.737710000 0.007830000 XXXX 1 xx Au 0.000

Au6 6.499780000 1.582980000 0.016490000 XXXX 1 xx Au 0.000

Au7 3.267700000 1.612470000 2.954390000 XXXX 1 xx Au 0.000

Au8 -0.000280000 4.775310000 2.950210000 XXXX 1 xx Au 0.000

LiZn

PBC 4.2409 4.6574 7.5384 79.6117 73.9630 62.9710 (P1)

Li1 1.754020000 0.982450000 4.805860000 XXXX 1 xx Li 0.000

Li2 3.937550000 0.169410000 0.364810000 XXXX 1 xx Li 0.000

Li3 3.832720000 2.392210000 3.925060000 XXXX 1 xx Li 0.000

Li4 3.912210000 2.727870000 1.243540000 XXXX 1 xx Li 0.000

Zn5 5.922490000 3.821560000 3.045210000 XXXX 1 xx Zn 0.000

Zn6 5.931390000 3.534750000 5.701010000 XXXX 1 xx Zn 0.000

Zn7 1.793940000 1.281060000 2.125560000 XXXX 1 xx Zn 0.000

Zn8 3.899930000 2.059590000 6.606110000 XXXX 1 xx Zn 0.000

LiAl

PBC 4.5860 4.5873 7.9168 106.6059 106.6821 60.2866 (P1)

Li1 1.983090000 0.029790000 6.046020000 XXXX 1 xx Li 0.000

Li2 1.962120000 2.622290000 2.375080000 XXXX 1 xx Li 0.000

Li3 1.974340000 0.022370000 3.297220000 XXXX 1 xx Li 0.000

Li4 -0.270060000 1.333380000 6.967760000 XXXX 1 xx Li 0.000

Al5 1.969370000 0.015450000 0.538060000 XXXX 1 xx Al 0.000

Al6 4.217560000 1.326220000 4.209960000 XXXX 1 xx Al 0.000

Al7 1.966690000 2.629730000 5.129800000 XXXX 1 xx Al 0.000

Al8 4.210980000 1.318590000 1.459500000 XXXX 1 xx Al 0.000

LiAs

PBC 5.8855 7.7079 7.9561 114.4860 70.9441 110.7929 (P1)

Li1 1.859470000 0.922990000 4.623440000 XXXX 1 xx Li 0.000

Li2 4.897390000 3.106130000 2.779800000 XXXX 1 xx Li 0.000

Li3 1.984670000 3.256160000 2.942870000 XXXX 1 xx Li 0.000

Li4 4.769830000 0.778910000 4.460330000 XXXX 1 xx Li 0.000

Li5 -0.812970000 5.458040000 1.083600000 XXXX 1 xx Li 0.000

Li6 4.659750000 -1.555250000 6.121530000 XXXX 1 xx Li 0.000

Li7 7.569630000 -1.434690000 6.319050000 XXXX 1 xx Li 0.000

Li8 2.102980000 5.583960000 1.265950000 XXXX 1 xx Li 0.000

As9 0.398580000 5.437510000 3.673450000 XXXX 1 xx As 0.000

As10 0.648570000 0.950380000 2.032670000 XXXX 1 xx As 0.000

As11 3.499420000 3.125260000 5.336770000 XXXX 1 xx As 0.000

As12 6.356490000 -1.400300000 3.722940000 XXXX 1 xx As 0.000

As13 3.381090000 3.227570000 0.390020000 XXXX 1 xx As 0.000

As14 3.256020000 0.909380000 2.059480000 XXXX 1 xx As 0.000

As15 0.277410000 3.107650000 5.349540000 XXXX 1 xx As 0.000

As16 0.775180000 3.273350000 0.358280000 XXXX 1 xx As 0.000

LiGe

PBC 2.8290 8.8187 5.9513 109.3845 90.0057 90.0256 (P1)

Li1 1.807200000 2.824930000 4.348370000 XXXX 1 xx Li 0.000

Li2 1.811230000 -0.999010000 2.976160000 XXXX 1 xx Li 0.000

Li3 1.807820000 3.767120000 1.716150000 XXXX 1 xx Li 0.000

Li4 1.811120000 -0.071790000 0.340920000 XXXX 1 xx Li 0.000

Ge5 0.408970000 0.446880000 4.986230000 XXXX 1 xx Ge 0.000

Ge6 0.409500000 1.379540000 2.342310000 XXXX 1 xx Ge 0.000

Ge7 0.406810000 6.147020000 1.076830000 XXXX 1 xx Ge 0.000

Ge8 0.406980000 5.211680000 3.718070000 XXXX 1 xx Ge 0.000

LiAg

PBC 4.7514 9.5878 3.0918 90.1608 90.0274 90.5529 (P1)

Li1 1.894650000 8.059320000 0.233530000 XXXX 1 xx Li 0.000

Li2 4.187040000 5.597370000 0.192780000 XXXX 1 xx Li 0.000

Li3 4.084580000 0.939610000 0.148580000 XXXX 1 xx Li 0.000

Li4 1.681920000 3.404150000 0.135950000 XXXX 1 xx Li 0.000

Ag5 3.997080000 3.261730000 1.627930000 XXXX 1 xx Ag 0.000

Ag6 4.234090000 7.918620000 1.730640000 XXXX 1 xx Ag 0.000

Ag7 1.738800000 1.076530000 1.652080000 XXXX 1 xx Ag 0.000

Ag8 1.869810000 5.731010000 1.677480000 XXXX 1 xx Ag 0.000