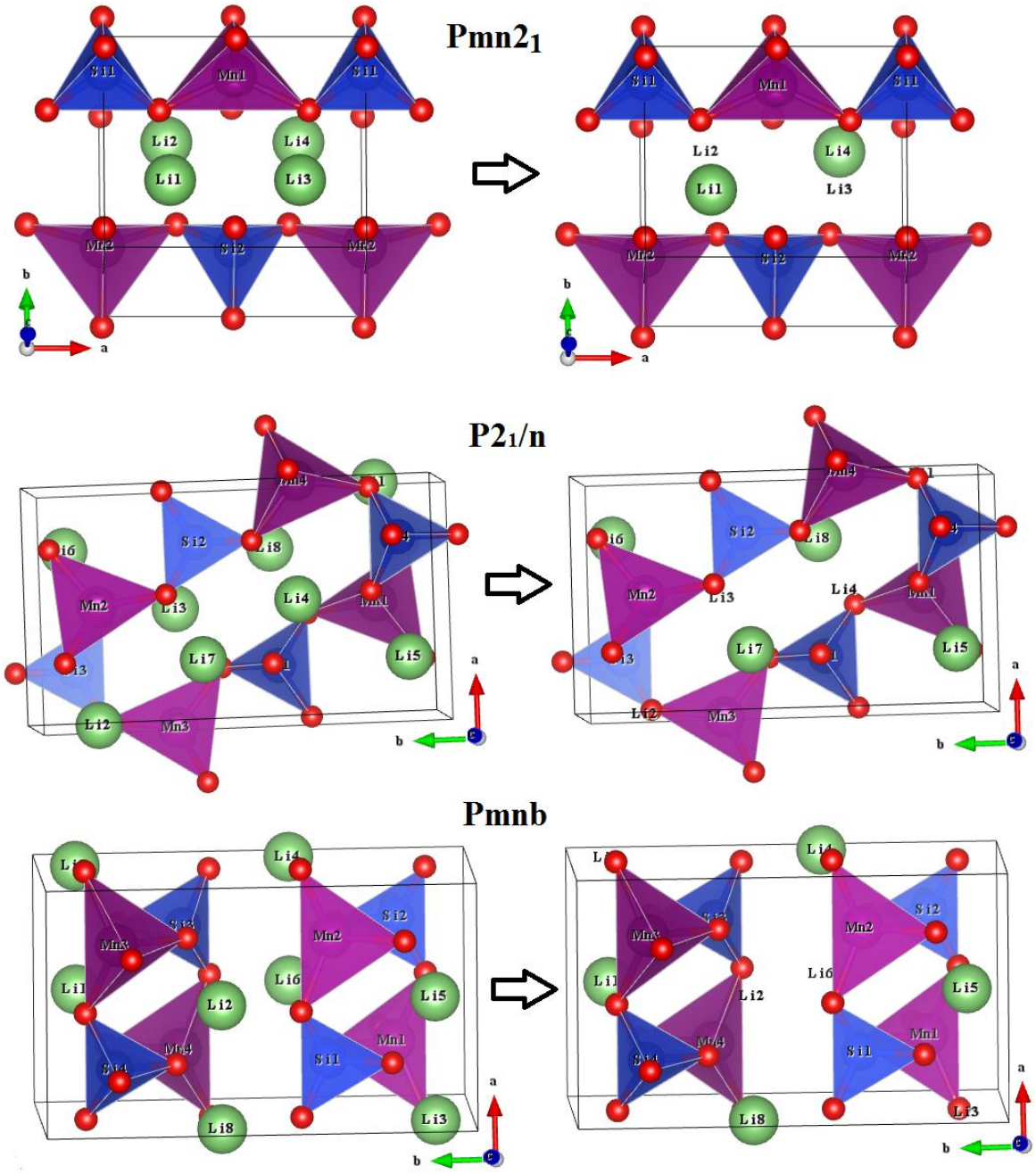

Fig. S1. Calculated the most stable configuration of delithiated structures ($LiMnSiO_4$) for three polymorphs after (right) and before (left) delithiation. For each structure there are three possible configurations for $LiMnSiO_4$ crystal, that the most stable ones were used as delithiated structures.

Table S1. k-points based on Monkhorst–Pack (MP) mesh as well as k-points in the irreducible Brillouin zone (iBz) for calculations of lithiated (Li2MnSiO4) and delithiated (LiMnSiO4 and MnSiO4) structures. In this table, space groups (S.G.) of the structure before lithium extraction (initial S.G.) and after

extraction of one lithium per formula (LiMnSiO4 S.G.) are also given. The S.G. after extraction of all Li atoms is equal to initial S.G.

initial S.G.	structure	$LiMnSiO_4$ S.G.	MP mesh	iBz
$Pmn2_1$	Li_2MnSiO_4	$Pmn2_1$	4×5×5	18
	$LiMnSiO_4$	P	4×5×5	50
	$MnSiO_4$	$Pmn2_1$	4×5×5	18
$P2_1/n$	Li_2MnSiO_4	$P2_1/n$	5×2×6	15
	$LiMnSiO_4$	$P2_1/n$	5×2×6	15
	$MnSiO_4$	$P2_1/n$	5×2×6	15
Pmnb	Li_2MnSiO_4	Pmnb	3×5×6	18
	$LiMnSiO_4$	$P2_1/c$	5×8×2	20
	$MnSiO_4$	Pmnb	3×5×6	18

Table S2. Lattice parameters, space group and atomic positions of Li_2MnSiO_4-$Pmn2_1$ structure calculated via PBE-GGA method.

a b c (Å)	6.3185	5.3865	4.9754
α β γ	90	90	90
space group:		Pmn21	
atom	x/a	y/b	z/c
Li	0.25215	0.32761	0.974766
Mn	0.5	0.822498	0.978927
Si	0	0.839622	0.985319
O 1	0.214367	0.689806	0.884504
O 2	0	0.131353	0.875499
O 3	0.5	0.153025	0.818214

Table S3. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4-$Pmn2_1$ structure ($LiMnSiO_4$) calculated via PBE-GGA method.

a b c (Å)	6.317881	5.370523	4.982241
α β γ	90	90	90
space group:		P	
atom	x/a	y/b	z/c
Li	0.74787	0.331669	0.975725
Li	0.24797	0.668385	0.475684
Mn	0.5019	0.827703	0.980109

Mn	0.00174	0.172511	0.480685
Si	0.99976	0.839387	0.984017
Si	0.49971	0.16032	0.483911
O	0.22325	0.697305	0.886807
O	0.99734	0.129323	0.860755
O	0.50205	0.138321	0.820974
O	0.72296	0.302711	0.386835
O	0.77611	0.693682	0.891917
O	0.27635	0.306341	0.392004
O	0.49734	0.870428	0.360505
O	0.00203	0.861538	0.320761

Table S4. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4-$Pmn2_1$ structure ($MnSiO_4$) calculated via PBE-GGA method.

a b c (Å)	6.304094	5.374115	4.985574
α β γ	90	90	90
space group:		Pmn21	
atom	x/a	y/b	z/c
Mn	0.5	0.830512	0.983327
Si	0	0.840415	0.984816
O 1	0.234118	0.711214	0.904512
O 2	0	0.12631	0.846223
O 3	0.5	0.129988	0.823638

Table S5. Lattice parameters, space group and atomic positions of Li_2MnSiO_4-$Pmn2_1$ structure calculated via LSDA method.

a b c (Å)	6.324034	5.391113	5.001343
α β γ	90	90	90
space group:		Pmn21	
atom	x/a	y/b	z/c
Li	0.247969	0.339384	0.932783
Mn	0.5	0.808672	0.974629
Si	0	0.853602	0.002768
O 1	0.214445	0.697952	0.919708
O 2	0	0.13408	0.867769
O 3	0.5	0.137202	0.834205

Table S6. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4-$Pmn2_1$ structure ($LiMnSiO_4$) calculated via LSDA method.

a b c (Å)	6.316034	5.387877	5.001343
α β γ	90	90	90
space group:		P	
atom	x/a	y/b	z/c
Li	0.244167	0.658934	0.456289
Li	0.744148	0.341082	0.956285
Mn	0.504378	0.805398	0.980701
Mn	0.004338	0.194546	0.480704
Si	0.998635	0.865391	0.985278
Si	0.498579	0.134619	0.485288
O	0.224353	0.738081	0.896798
O	0.971276	0.136371	0.836522
O	0.528599	0.097215	0.811819
O	0.724299	0.261925	0.396894
O	0.780561	0.699216	0.955918
O	0.280533	0.300811	0.455994
O	0.471353	0.86363	0.336505
O	0.028552	0.902712	0.311822

Table S7. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4-$Pmn2_1$ structure ($MnSiO_4$) calculated via LSDA method.

a b c (Å)	6.319816	5.387517	4.998007
α β γ	90	90	90
space group:		Pmn21	
atom	x/a	y/b	z/c
Mn	0.5	0.819499	0.986335
Si	0	0.851771	0.999664
O 1	0.231076	0.718272	0.92906
O 2	0	0.128229	0.848698
O 3	0.5	0.117333	0.837364

Table S8. Lattice parameters, space group and atomic positions of Li_2MnSiO_4-$P2_1/n$ structure calculated via PBE-GGA method.

a b c (Å)	6.3156	10.8812	5.0602
α β γ	90	90.987	90
space group:		P21/n	
atom	x/a	y/b	z/c
Mn	0.495679	0.165508	0.309196
Si	0.242714	0.410462	0.304826

Li1	0.996781	0.161769	0.304351
Li2	0.241774	0.074346	0.70711
O 1	0.23862	0.410169	0.632245
O 2	0.248318	0.553239	0.193347
O 3	0.026726	0.337041	0.200016
O 4	0.461139	0.339427	0.209495

Table S9. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- $P2_1/n$ structure ($LiMnSiO_4$) calculated via PBE-GGA method.

a b c (Å)	6.293148	10.7981	5.036036
α β γ	90	90.987	90
space group:		P21/n	
atom	x/a	y/b	z/c
Li2	0.237254	0.074735	0.703418
Mn	0.493041	0.166137	0.314414
Si	0.240579	0.409715	0.307322
O 1	0.219648	0.407687	0.633939
O 2	0.236431	0.553533	0.197131
O 3	0.028533	0.340947	0.180072
O 4	0.458544	0.332831	0.221836

Table S10. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- $P2_1/n$ structure ($MnSiO_4$) calculated via PBE-GGA method.

a b c (Å)	6.214295	10.70109	5.001647
α β γ	90	90.987	90
space group:		P21/n	
atom	x/a	y/b	z/c
Si	0.243125	0.41072	0.306218
O 1	0.217338	0.403366	0.638212
O 2	0.23237	0.557381	0.202603
O 3	0.03257	0.338243	0.172276
O 4	0.458119	0.328059	0.221653

Table S11. Lattice parameters, space group and atomic positions of Li_2MnSiO_4- $P2_1/n$ structure calculated via LSDA method.

a b c (Å)	6.314812	10.8781	5.056036
α β γ	90	90.987	90

space group:		P21/n	
atom	x/a	y/b	z/c
Li1	0.990866	0.161214	0.303483
Li2	0.243839	0.072948	0.704248
Mn	0.491414	0.166475	0.307529
Si	0.236548	0.408275	0.298656
O 1	0.22746	0.408885	0.623668
O 2	0.241924	0.550166	0.184777
O 3	0.023594	0.33493	0.189522
O 4	0.455753	0.337628	0.207943

Table S12. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- $P2_1/n$ structure ($LiMnSiO_4$) calculated via LSDA method.

a b c (Å)	6.251022	10.76821	5.004961
α β γ	90	90.987	90
space group:		P21/n	
atom	x/a	y/b	z/c
Li2	0.215281	0.068902	0.688859
Mn	0.461619	0.171483	0.320762
Si	0.207072	0.409481	0.316667
O 1	0.162483	0.41143	0.63511
O 2	0.238138	0.549859	0.202987
O 3	0.001496	0.342512	0.17381
O 4	0.430638	0.336056	0.260399

Table S13. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- $P2_1/n$ structure ($MnSiO_4$) calculated via LSDA method.

a b c (Å)	6.096884	10.50269	4.881549
α β γ	90	90.987	90
space group:		P21/n	
atom	x/a	y/b	z/c
Mn	0.491414	0.166475	0.307529
Si	0.236548	0.408275	0.298656
O 1	0.22746	0.408885	0.623668
O 2	0.241924	0.550166	0.184777
O 3	0.023594	0.33493	0.189522
O 4	0.455753	0.337628	0.207943

Table S14. Lattice parameters, space group and atomic positions of Li_2MnSiO_4-Pmnb structure calculated via PBE-GGA method.

a b c (Å)	6.334973	10.83638	5.056433
α β γ	90	90	90
space group:		Pmnb	
atom	x/a	y/b	z/c
Li	0.500643	0.088466	0.316171
Mn	0.25	0.830902	0.184075
Si	0.25	0.662738	0.675752
O 1	0.25	0.663282	0.348556
O 2	0.963252	0.902014	0.275486
O 3	0.25	0.808896	0.781312

Table S15. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- Pmnb structure ($LiMnSiO_4$) calculated via PBE-GGA method.

a b c (Å)	8.100109	5.05306	10.82915
α β γ	90	90	128.5961
space group:		P21/c	
atom	x/a	y/b	z/c
Li	0.683224	0.998906	0.588028
Mn	0.079169	0.26011	0.329094
Si	0.57149	0.246716	0.166565
O 1	0.911677	0.25429	0.172359
O 2	0.252078	0.520084	0.398968
O 3	0.301518	0.026147	0.597399
O 4	0.44769	0.246587	0.309747

Table S16. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- Pmnb structure ($MnSiO_4$) calculated via PBE-GGA method.

a b c (Å)	6.330747	10.82915	5.05306
α β γ	90	90	90
space group:		Pmnb	
atom	x/a	y/b	z/c
Mn	0.25	0.828409	0.182025
Si	0.25	0.665487	0.675561
O 1	0.25	0.672228	0.340618
O 2	0.988703	0.897508	0.26565
O 3	0.25	0.8088	0.801503

Table S17. Lattice parameters, space group and atomic positions of Li_2MnSiO_4- Pmnb structure calculated via LSDA method.

a b c (Å)	6.313571	10.79977	5.03935
α β γ	90	90	90
space group:		Pmnb	
atom	x/a	y/b	z/c
Li	0.500906	0.08821	0.316858
Mn	0.25	0.830925	0.184744
Si	0.25	0.664003	0.675138
O 1	0.25	0.664755	0.346933
O 2	0.971781	0.90067	0.276165
O 3	0.25	0.808397	0.784217

Table S18. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- Pmnb structure ($LiMnSiO_4$) calculated via LSDA method.

a b c (Å)	8.072744	5.035988	10.79256
α β γ	90	90	128.5961
space group:		P21/c	
atom	x/a	y/b	z/c
Li	0.682628	0.498993	0.088324
Mn	0.074233	0.757806	0.829566
Si	0.571117	0.746026	0.666062
O 1	0.909161	0.752845	0.670276
O 2	0.250164	0.020376	0.897656
O 3	0.700463	0.47618	0.901012
O 4	0.451814	0.747596	0.809119

Table S19. Lattice parameters, space group and atomic positions of delithiated Li_2MnSiO_4- Pmnb structure ($MnSiO_4$) calculated via LSDA method.

a b c (Å)	6.30936	10.79256	5.035988
α β γ	90	90	90
space group:		Pmnb	
atom	x/a	y/b	z/c
Mn	0.25	0.829417	0.18368
Si	0.25	0.66494	0.675747
O 1	0.25	0.670727	0.342593

O 2	0.985747	0.89611	0.267223
O 3	0.25	0.80833	0.797859