

Electronic supplementary information (ESI)

Determination of Possible Configurations for $\text{Li}_{0.5}\text{CoO}_2$ a Delithiated Li-Ion Battery Cathodes via DFT Calculation Coupled with a Multi-Objective Non-Dominated Sorting Genetic Algorithm (NSGA-III)

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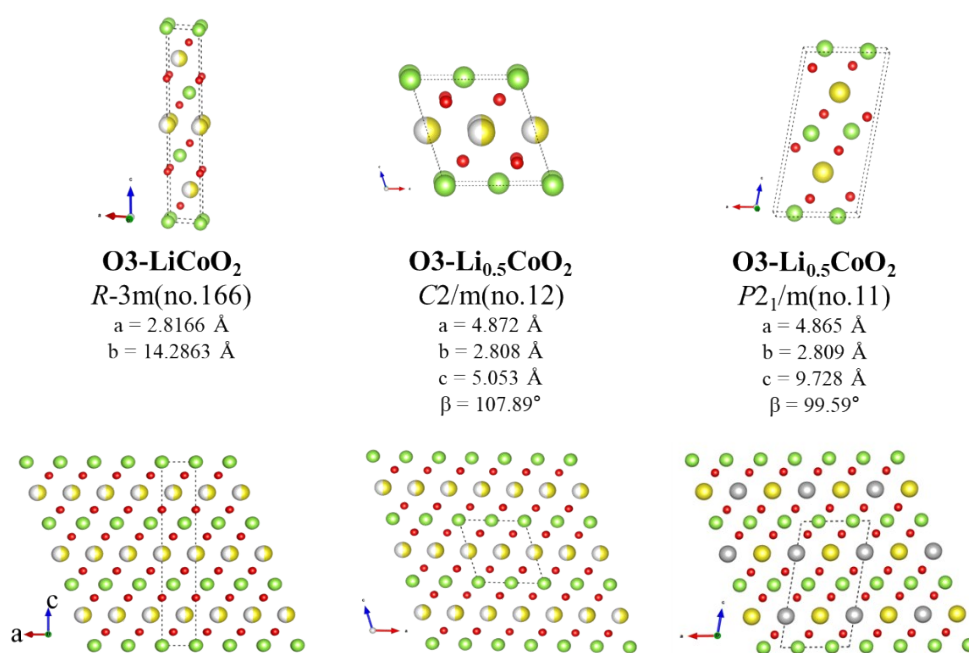


Fig. S1 Three known structures of Li_{0.5}CoO₂; the first row stands for conventional unit cell representations based on the conventional symmetry and periodicity and the bottom row for apparent look (the conventional unit cell is depicted inside).

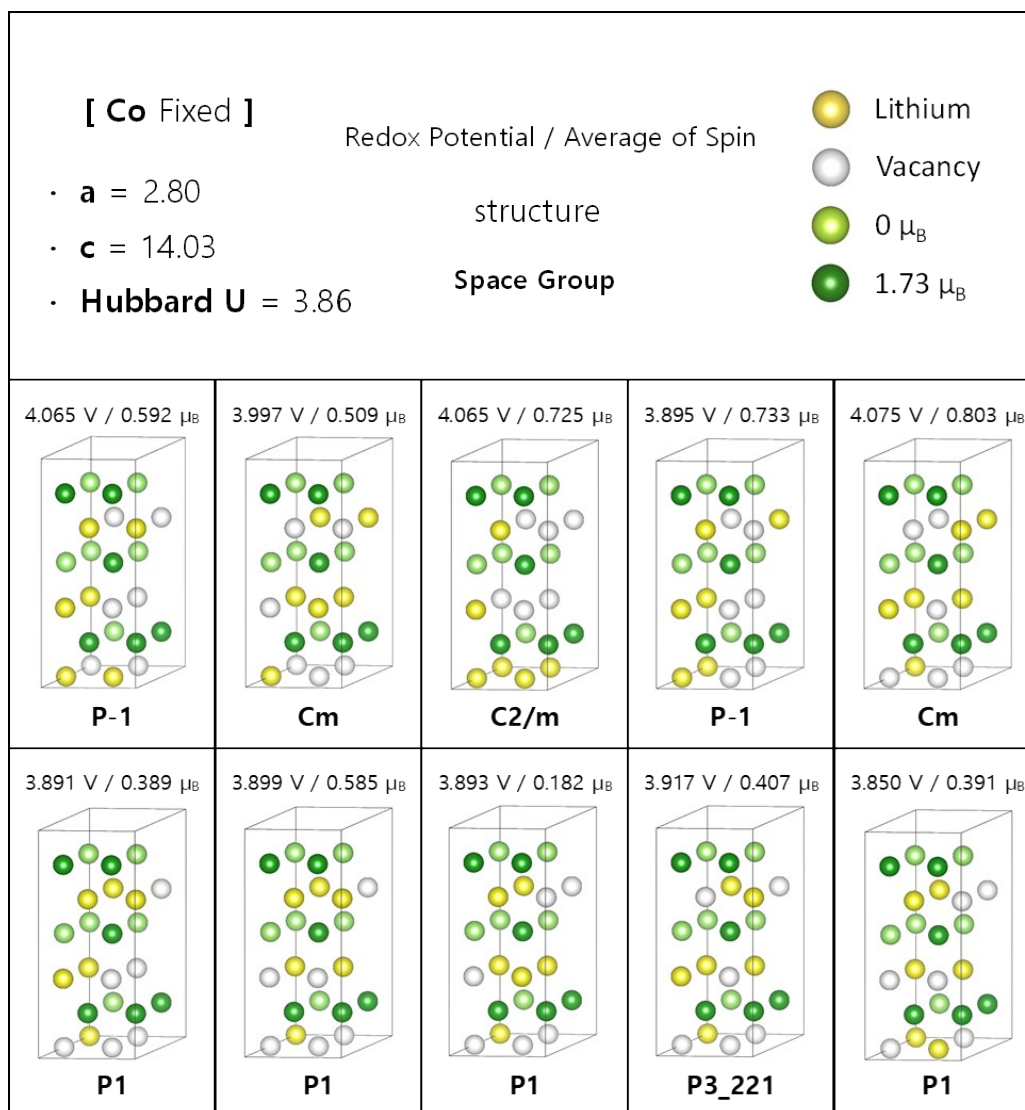


Fig. S2 The effect of the Li/V_{Li} configuration on the redox potential and the magnetic moment. The values were calculated with all other decision variables and hyper-parameters fixed.

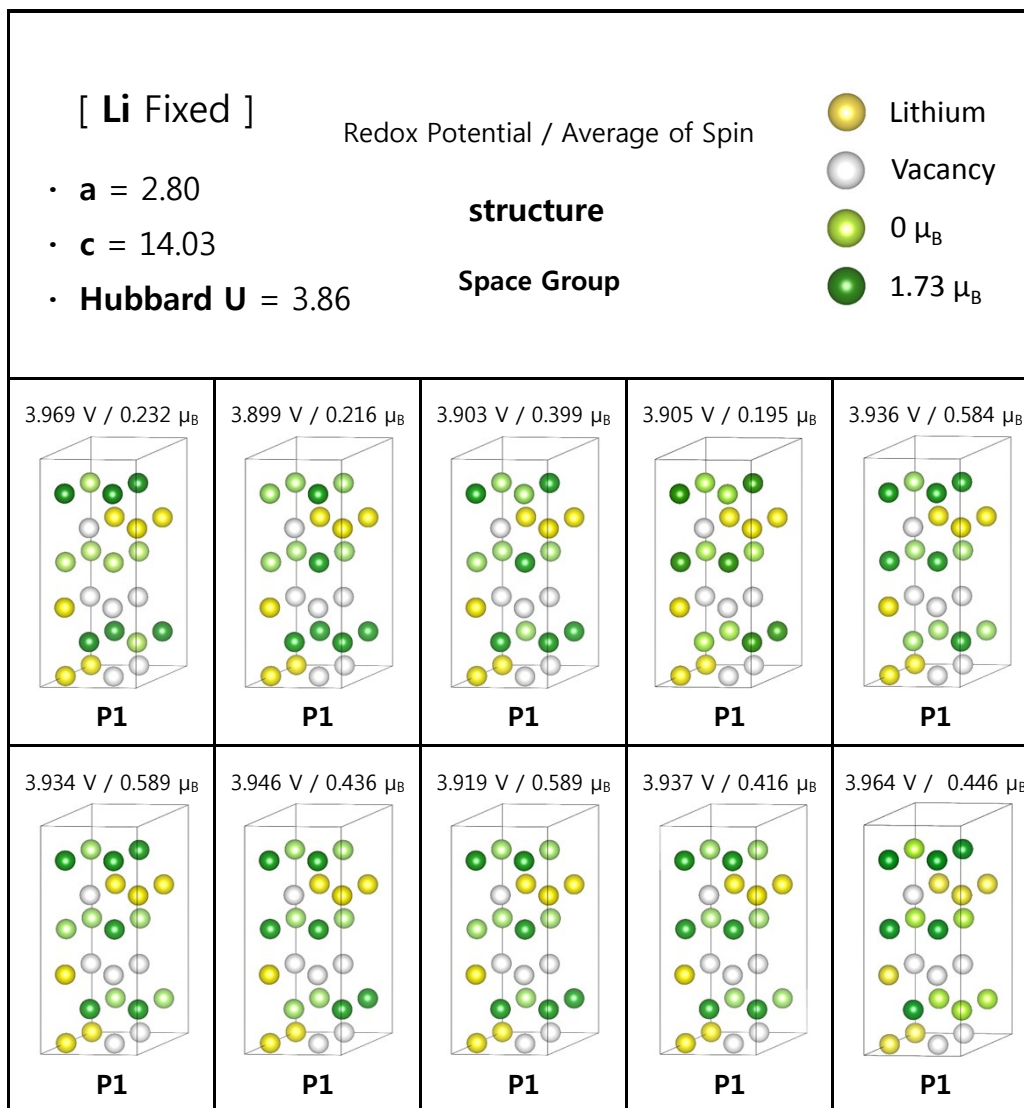


Fig. S3 The effect of the $\text{Co}^{3+}/\text{Co}^{4+}$ configuration on the redox potential and the magnetic moment were calculated with all other decision variables and hyper-parameters fixed.

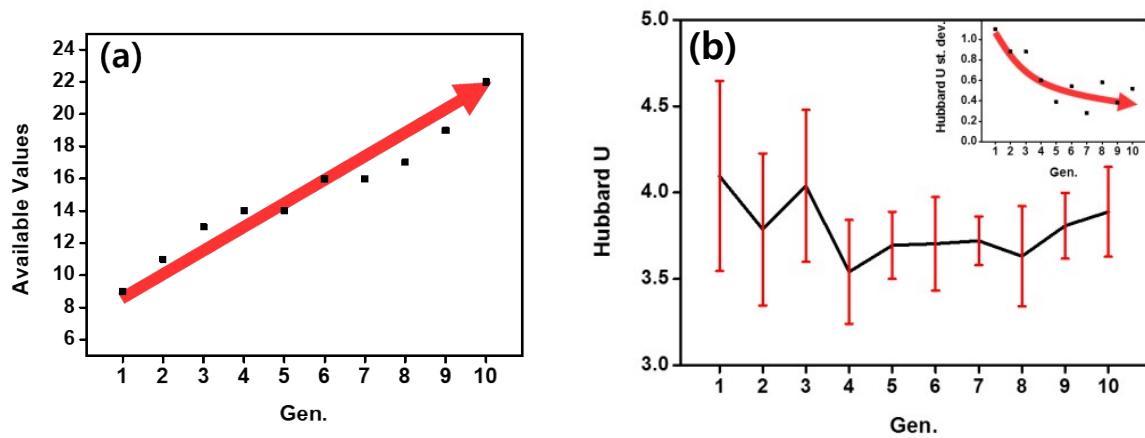
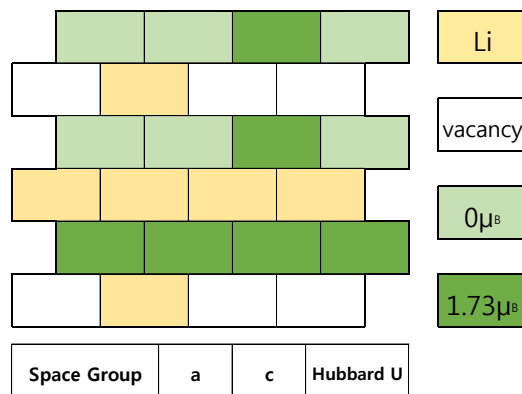


Fig. S4 The conventional 1-D plot of the objective functions and some other important parameters vs. the generation number. (a) the number of converged entries increases as the evolution goes on to later generations. Although we did not discuss this in the manuscript, this plot is indicative of a clear evidence for effective evolution. The random nature of the first generation made many entries in the first generation lead to failures in convergence, but most of entries survived in the last generation. (b) the average Hubbard U value for each generation as a function of the generation number. A definite evolution trend is obvious, that is, the average U value slightly decrease as the generation number increases and converged slightly below 4 eV. Because we designed the search space for Hubbard U around a generally known value in order to avoid futile computation burdens, Hubbard U converged so early. More importantly than the average U value, the standard deviation showed a more dramatic evolution, i.e., the standard deviation definitely decreases as the generation number increases, as shown in the inset to Fig. S4 (b). The first three generations show very high standard deviation but the evolution took place in the direction of decreasing it.

An example of the structure



1st Gen.					
1 Cm 2.72 14.15 5.88	2 Cm 2.75 14.17 3.00	3 Cm 2.82 14.01 4.05	4 P3_121 2.90 13.91 4.35	5 P1 2.73 14.19 5.61	6 C2/m 2.79 13.90 5.68
7 P1 2.74 14.12 2.72	8 P-1 2.81 13.96 3.43	9 P-1 2.71 14.13 4.08	10 P-1 2.90 13.90 5.26	11 P3_221 2.71 14.18 2.33	12 Cm 2.74 14.17 3.2
13 Cm 2.81 14.16 4.67	14 Cm 2.71 14.11 2.52	15 C2/m 2.70 14.18 5.83	16 P1 2.90 13.91 3.42	17 Cm 2.85 13.91 3.42	18 P-1 2.82 14.14 4.36
19 P3_221 2.72 14.19 5.23	20 P3_121 2.87 14.02 3.45	21 Pm 2.84 13.91 4.87	22 P-1 2.75 14.15 3.03	23 P1 2.78 14.15 5.07	24 P2/m 2.85 13.90 3.06
25 Cm 2.71 14.19 4.02	26 P1 2.89 13.92 4.40	27 P-3m1 2.90 13.96 5.16	28 P1 2.83 13.90 2.57		

2nd Gen.					
1 P-1 2.81 14.17 3.8	2 Cm 2.71 14.18 2.82	3 Pm 2.78 14.06 4.05	4 Cm 2.88 13.91 4.28	5 Cm 2.77 14.06 5.80	6 Cm 2.77 14.10 2.98
7 P3_221 2.81 14.06 3.96	8 P1 2.82 14.01 3.85	9 C2/m 2.74 14.11 2.76	10 P1 2.74 14.04 2.94	11 C2/m 2.86 14.07 3.30	12 P1 2.84 14.11 3.61
13 P3_221 2.76 14.17 2.70	14 Cm 2.75 14.07 4.08	15 Cm 2.87 13.92 3.54	16 P3_121 2.83 14.02 5.29	17 Cm 2.74 14.06 3.88	18 P1 2.87 13.90 4.18
19 P2/m 2.80 13.96 4.03	20 P1 2.72 14.14 2.79	21 Cm 2.86 14.05 2.81	22 P1 2.81 14.05 3.36	23 C2/m 2.90 13.96 5.16	24 P3_221 2.72 14.19 5.60
25 P-1 2.85 13.90 3.06	26 P1 2.82 14.11 3.80	27 Cm 2.86 14.12 2.44	28 P-1 2.87 13.90 5.26	29 P-1 2.90 13.90 4.85	30 P-1 2.71 14.13 3.87

3rd Gen.					
1 C2/m 2.77 13.93 3.54	2 P-1 2.76 14.13 3.12	3 P1 2.85 13.90 5.47	4 Cm 2.87 13.90 5.47	5 Cm 2.75 14.07 4.16	6 P-1 2.81 14.12 4.29
7 P-1 2.79 14.03 3.84	8 Cm 2.75 14.05 3.83	9 P1 2.80 14.16 5.05	10 P1 2.83 14.11 2.83	11 Cm 2.77 14.08 3.71	12 Pm 2.83 14.17 3.9
13 P1 2.76 14.01 2.87	14 P-1 2.80 13.90 5.47	15 C2/m 2.86 14.12 4.69	16 P-1 2.76 14.08 5.78	17 Cm 2.80 14.04 4.62	18 Cm 2.75 13.92 5.08
19 Pm 2.77 14.13 3.4	20 P1 2.72 14.07 3.76	21 P1 2.82 14.12 4.13	22 Cm 2.75 14.10 3.52	23 Cm 2.84 14.10 3.72	24 Cm 2.72 14.11 5.88
25 P1 2.81 14.04 3.61	26 P1 2.86 13.9 3.77	27 Cm 2.83 14.06 3.29	28 P-1 2.81 14.14 4.38	29 P-1 2.71 14.13 3.87	30 P1 2.83 13.87 2.57

4th Gen.					
1 Cm 2.79 14.04 3.50	2 P-3m1 2.80 14.09 4.25	3 P2/m 2.81 14.11 4.38	4 C2/m 2.80 14.00 3.07	5 P1 2.87 13.91 3.34	6 P1 2.85 14.16 2.57
7 P3_121 2.81 14.12 3.40	8 P1 2.85 14.08 3.21	9 Cm 2.80 14.08 2.98	10 Cm 2.88 13.91 3.16	11 P-1 2.87 14.14 4.21	12 P-1 2.73 14.09 3.83
13 C2/m 2.82 14.15 4.00	14 Pm 2.85 13.92 3.85	15 P-1 2.81 14.00 3.16	16 P1 2.86 13.90 2.65	17 P2/m 2.84 14.13 3.78	18 P-1 2.73 14.06 3.97
19 P1 2.84 14.07 2.89	20 Cm 2.75 14.01 2.74	21 C2/m 2.84 13.90 2.83	22 C2/m 2.82 13.93 4.26	23 P-1 2.82 13.96 2.84	24 P2/m 2.72 14.18 3.15
25 P-1 2.77 13.93 3.54	26 P1 2.81 14.06 3.96	27 Pm 2.83 14.18 3.90	28 P1 2.80 14.23 5.05	29 P-1 2.71 14.13 3.87	30 P1 2.72 14.07 3.90

5th Gen.					
1 P-1 2.77 14.13 3.79	2 Cm 2.84 14.11 3.74	3 Cm 2.87 14.08 3.39	4 Cm 2.81 13.97 3.99	5 Cm 2.80 14.07 3.83	6 P1 2.80 13.93 3.28
7 P1 2.72 14.10 3.33	8 P1 2.72 14.18 3.89	9 P-1 2.82 14.00 3.29	10 Cm 2.73 14.15 4.18	11 P1 2.81 14.15 3.93	12 P3 121 2.78 14.01 4.25
13 P-1 2.87 13.97 4.16	14 P-1 2.81 13.96 3.34	15 P-1 2.78 14.10 3.81	16 P-1 2.83 14.05 3.16	17 Pm 2.82 14.10 3.83	18 P1 2.81 14.06 3.68
19 Cm 2.81 14.08 3.94	20 P-1 2.83 14.00 3.16	21 Cm 2.74 14.07 3.78	22 Cm 2.85 14.02 4.58	23 C2/m 2.80 13.93 4.26	24 P1 2.88 13.90 3.15
25 Cm 2.81 14.05 3.96	26 P1 2.75 14.01 4.10	27 P1 2.80 13.99 3.16	28 Cm 2.83 13.97 3.52	29 P-1 2.79 14.1 3.63	30 Pm 2.80 14.1 3.50

6th Gen.					
1 	2 	3 	4 	5 	6
7 	8 	9 	10 	11 	12
13 	14 	15 	16 	17 	18
19 	20 	21 	22 	23 	24
25 	26 	27 	28 	29 	30

7th Gen.					
1 	2 	3 	4 	5 	6
7 	8 	9 	10 	11 	12
13 	14 	15 	16 	17 	18
19 	20 	21 	22 	23 	24
25 	26 	27 	28 	29 	30

8th Gen.					
1 P-1 2.81 13.96 3.47	2 P1 2.82 13.97 3.50	3 Cm 2.80 14.02 4.33	4 P3_221 2.80 14.09 4.34	5 Cm 2.85 14.08 3.80	6 Cm 2.80 14.07 3.53
7 P1 2.82 14.15 4.54	8 P1 2.83 14.07 3.77	9 P-1 2.81 14.06 3.85	10 P1 2.79 13.96 3.32	11 P1 2.76 14.07 3.78	12 P1 2.79 13.99 3.09
13 Cm 2.80 13.95 3.15	14 P-1 2.80 14.09 3.32	15 Cm 2.80 14.16 4.66	16 P1 2.79 14.04 3.16	17 P1 2.79 14.08 3.58	18 P3_121 2.81 14.15 4.29
19 Cm 2.80 14.02 3.18	20 P1 2.80 14.03 3.86	21 Cm 2.80 14.07 3.23	22 Cm 2.83 14.02 5.29	23 P1 2.80 13.95 3.05	24 Cm 2.79 14.03 3.59
25 Cm 2.85 14.00 3.12	26 P1 2.76 14.03 3.81	27 Cm 2.85 14.05 2.70	28 P1 2.79 14.06 3.03	29 Cm 2.79 14.04 3.59	30 Cm 2.80 14.02 3.03

9th Gen.					
1 Cm 2.80 14.04 3.56	2 P-1 2.79 14.08 3.13	3 P1 2.83 14.05 3.92	4 P-3m1 2.85 14.00 4.12	5 Cm 2.80 14.13 3.43	6 Cm 2.86 14.00 4.14
7 P-1 2.78 14.10 3.95	8 P1 2.80 14.09 3.69	9 P3_121 2.78 14.10 3.81	10 Cm 2.81 14.03 3.58	11 Cm 2.81 14.14 3.71	12 Cm 2.71 14.13 4.08
13 P1 2.81 14.10 3.92	14 Cm 2.80 14.11 4.06	15 P1 2.8 14.11 3.70	16 Cm 2.8 14.08 4.4	17 P1 2.80 14.02 3.64	18 Cm 2.83 14.07 3.77
19 Cm 2.87 14.08 3.8	20 Pm 2.79 14.03 3.59	21 P1 2.85 14.08 3.80	22 Cm 2.79 14.03 3.59	23 P-1 2.81 14.17 4.36	24 Cm 2.82 14.15 4.54
25 Cm 2.79 14.03 4.53	26 P1 2.84 14.12 4.42	27 Cm 2.81 13.95 3.01	28 P1 2.80 14.07 3.06	29 Cm 2.79 14.07 3.22	30 P1 2.83 14.07 3.77



Fig. S5 Schematics of the configurations represented along with other decision variables for each generation.

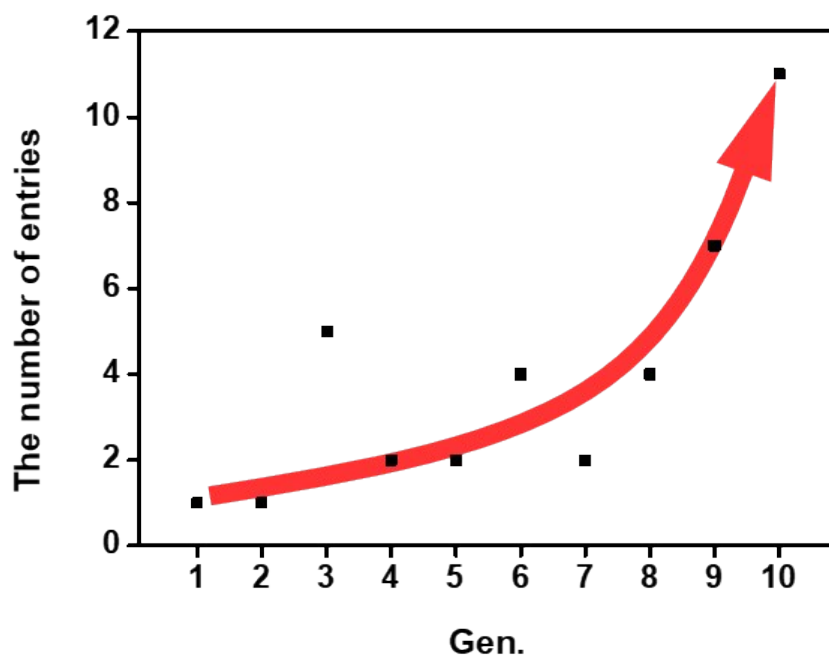


Fig. S6 Plot of the number of entries vs. the generation number. This plot indicates the classification of the finally selected 39 entries in terms of the generation from which each entry originated.

Table S1 The Effect of the initial input lattice parameters on the relaxed lattice parameter, the total energy, and the average $\Delta\mu$ was examined with all other decision variables and hyper-parameters fixed.

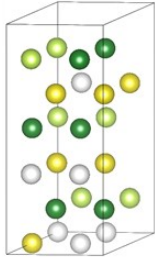
Fixed - Hubbard $U = 3.86$ - Space Group : Cm   Lithium  Vacancy  $0 \mu_B$  $1.73 \mu_B$						
No.	Input		Calculated			
	Initial		Relaxed		μ_{average}	E_{total}
	a	c	a	c		
1	2.750	13.900	2.821	14.667	0.186	-22744.818
2	2.750	14.030	2.818	14.607	0.007	-22756.932
3	2.750	14.100	2.818	14.616	0.200	-22751.910
4	2.800	13.900	2.819	14.495	0.676	-22687.104
5	2.800	14.030	2.822	14.531	0.583	-22727.076
6	2.800	14.100	2.817	14.565	0.581	-22718.322
7	2.865	13.900	2.826	14.533	0.506	-22678.302
8	2.865	14.030	2.848	14.585	0.733	-22573.902
9	2.865	14.100	2.830	14.571	0.652	-22623.036
10	2.795	14.100	2.818	14.559	0.601	-22545.408

Table S2. The objective function values and decision variables along with other calculated results for all generations. The lattice parameter and the average μ have duality either as an initial input or as a DFT-calculated result, so that we should consider them separately for a clearer understanding. Namely, we discerned between the initial preset input of μ and the DFT-calculated μ , and also between the initial preset of lattice parameters and the DFT-relaxed lattice parameters. Aside from the three objective functions the total energy is also listed. For convenience sake, it should be noted that the lattice parameters (a and c) are based on the R-3m supercell structure, rather than on the configuration-driven symmetry. The blanks in the table represent non-converged entries. The number of blanks decreases in later generations.

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
1	1	5.44	14.15	5.88	Cm	5.71	14.65	1.19	-21348.92	5.86	14.44	3.15	-24930.18	4.45	1.07	4.04
	2	5.49	14.17	3.00	Cm											
	3	5.65	14.01	4.05	Cm	5.66	14.70	0.83	-22585.10	5.76	14.30	1.92	-25495.25	3.29	0.00	2.45
	4	5.80	13.91	4.35	P3_121											
	5	5.47	14.19	5.61	P1											
	6	5.57	13.90	5.68	C2/m	5.71	14.71	1.58	-21473.06	5.82	14.50	3.14	-24962.32	4.29	0.00	4.42
	7	5.47	14.12	2.72	P1											
	8	5.63	13.96	3.43	P-1											
	9	5.42	14.13	4.08	P-1	5.65	14.79	0.29	-22592.86	5.82	14.36	2.17	-25381.08	3.08	0.00	2.19
	10	5.80	13.90	5.26	P-1	5.68	14.74	1.51	-21727.13	5.82	14.54	3.12	-25145.14	4.17	0.00	4.33
	11	5.41	14.18	2.33	P3_221											
	12	5.49	14.17	3.20	Cm											
	13	5.62	14.16	4.67	Cm	5.65	14.58	0.67	-22160.33	5.80	14.61	3.05	-24923.40	3.04	0.00	3.42
	14	5.43	14.11	2.52	Cm											
	15	5.41	14.18	5.83	C2/m											
	16	5.79	13.91	3.42	P1	5.65	14.66	0.75	-22959.37	5.75	14.53	2.56	-25583.34	2.80	0.00	3.01
	17	5.71	13.91	3.42	Cm											
	18	5.64	14.14	4.36	P-1	5.65	14.74	0.81	-22264.88	5.76	14.31	1.95	-25353.61	3.60	0.00	2.46
	19	5.43	14.19	5.23	P3_221											
	20	5.75	14.02	3.45	P3_121											
	21	5.69	13.91	4.87	Pm	5.78	14.50	1.34	-21847.85	5.79	14.47	3.11	-25291.72	4.22	1.78	4.15
	22	5.49	14.15	3.03	P-1											
	23	5.56	14.15	5.07	P1											
	24	5.70	13.90	3.06	P2/m											
	25	5.42	14.19	4.02	Cm											
	26	5.78	13.92	4.40	P1											
	27	5.80	13.96	5.16	P-3m1											
	28	5.66	13.90	2.57	P1											

Table S2 Continued

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
2	1	5.62	14.17	3.8	P-1	5.65	14.67	0.43	-22720.09	5.76	14.32	1.90	-25612.07	3.26	0.00	2.03
	2	5.42	14.18	2.82	Cm											
	3	5.56	14.06	4.05	Pm											
	4	5.76	13.91	4.28	Cm	5.65	14.64	0.49	-22430.71	5.79	14.47	3.09	-25502.69	3.57	0.72	3.28
	5	5.54	14.06	5.80	Cm											
	6	5.54	14.10	2.98	Cm											
	7	5.62	14.06	3.96	P3 221											
	8	5.65	14.01	3.85	P1	5.68	14.57	0.34	-22639.43	5.80	14.52	2.91	-25526.44	3.25	0.00	2.94
	9	5.48	14.11	2.76	C2/m											
	10	5.48	14.04	2.94	P1											
	11	5.72	14.07	3.30	C2/m	5.66	14.58	0.54	-23054.56	5.77	14.30	1.86	-25858.21	3.11	0.00	2.10
	12	5.66	14.10	4.05	P-1	5.65	14.59	0.65	-22652.89	5.85	14.49	2.74	-25521.50	3.22	0.00	3.10
	13	5.48	14.17	2.70	P3 221											
	14	5.50	14.07	4.08	Cm											
	15	5.74	13.92	3.54	Cm											
	16	5.68	14.11	3.61	P1	5.64	14.57	0.56	-22924.63	5.81	14.30	1.89	-25715.62	3.09	0.00	2.15
	17	5.48	14.06	3.88	Cm											
	18	5.74	13.90	4.18	P1	5.65	14.63	0.89	-22462.21	5.80	14.52	2.77	-25270.27	3.12	0.00	3.36
	19	5.60	13.96	4.03	P2/m											
	20	5.44	14.14	2.79	P1											
	21	5.72	14.05	2.81	Cm	5.63	14.59	0.50	-23494.41	5.67	14.09	0.00	-26679.97	3.77	1.78	0.20
	22	5.62	14.05	3.36	P1											
	23	5.80	13.96	5.16	C2/m											
	24	5.44	14.19	5.60	P3 221											
	25	5.70	13.90	3.06	P-1											
	26	5.64	14.11	3.80	P1	5.65	14.56	0.58	-22752.73	5.77	14.53	2.74	-25486.91	2.99	0.00	3.03
	27	5.72	14.12	2.44	Cm											
	28	5.74	13.90	5.26	P-1											
	29	5.80	13.90	4.85	P-1	5.70	14.69	0.97	-22001.10	5.80	14.47	3.11	-25307.56	3.98	0.72	3.78
	30	5.42	14.13	3.87	P-1	5.62	14.64	0.19	-22792.77	5.82	14.35	2.15	-25477.24	2.90	1.90	2.26

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
3	1	5.54	13.93	3.54	C2/m											
	2	5.52	14.13	3.12	P-1											
	3	5.70	13.90	5.47	P1	5.72	14.55	1.15	-21629.78	5.84	14.47	3.13	-25072.81	4.22	1.34	3.98
	4	5.74	13.90	3.01	Cm	5.63	14.55	0.32	-23342.60	5.67	14.10	0.00	-26547.88	3.80	1.79	0.02
	5	5.50	14.07	4.16	Cm											
	6	5.63	14.12	4.29	P-1	5.67	14.60	0.32	-22441.85	5.80	14.30	1.95	-25393.51	3.37	0.00	1.95
	7	5.59	14.03	3.84	P-1											
	8	5.50	14.05	3.83	Cm											
	9	5.60	14.16	5.05	P1											
	10	5.66	14.11	2.83	P1											
	11	5.54	14.08	3.71	Cm											
	12	5.66	14.17	3.90	Pm	5.64	14.60	0.58	-22649.40	5.88	14.46	3.08	-25593.46	3.35	0.52	3.36
	13	5.52	14.01	2.87	P1											
	14	5.60	13.90	5.47	P-1	5.68	14.68	0.73	-21663.91	5.81	14.44	3.13	-25064.18	4.14	1.34	3.56
	15	5.72	14.12	4.69	C2/m	5.71	14.36	1.13	-22066.85	5.88	14.47	3.11	-25317.60	3.88	1.13	3.93
	16	5.52	14.08	5.78	P-1											
	17	5.60	14.04	4.62	Cm	5.68	14.53	0.54	-22176.56	5.75	14.31	1.97	-25231.87	3.55	0.00	2.21
	18	5.50	13.92	5.08	Cm	5.68	14.74	0.73	-21857.00	5.79	14.50	3.12	-25237.45	4.11	0.92	3.54
	19	5.54	14.13	3.40	Pm											
	20	5.44	14.07	3.76	P1											
	21	5.64	14.12	4.13	P1	5.64	14.57	0.37	-22537.07	5.76	14.31	1.93	-25459.06	3.32	0.00	2.00
	22	5.50	14.10	3.52	Cm											
	23	5.66	14.10	3.72	Cm											
	24	5.44	14.11	5.88	Cm											
	25	5.62	14.04	3.61	P1											
	26	5.72	13.91	3.77	P1	5.67	14.55	0.39	-22718.02	5.76	14.29	1.90	-25629.91	3.30	0.00	1.99
	27	5.66	14.06	3.29	Cm											
	28	5.61	14.14	4.37	P-1	5.68	14.59	0.68	-22347.85	5.75	14.31	1.95	-25342.66	3.44	0.00	2.33
	29	5.42	14.13	3.87	P-1	5.62	14.56	0.02	-22790.24	5.82	14.36	2.15	-25477.24	2.91	1.90	2.43
	30	5.66	13.87	2.57	P1	5.63	14.53	0.31	-23678.55	5.67	14.07	0.00	-26835.04	3.72	1.58	0.01

Table S2 Continued

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
4	1	5.58	14.04	3.50	C2/m											
	2	5.61	14.09	4.25	P-3m1	5.65	14.60	0.58	-22418.60	5.76	14.31	1.94	-25400.88	3.42	0.00	2.22
	3	5.61	14.11	4.38	P2/m	5.65	14.75	0.68	-22338.47	5.76	14.31	1.95	-25342.25	3.46	0.00	2.33
	4	5.59	14.00	3.07	C2/m											
	5	5.73	13.91	3.34	P1	5.68	14.58	0.67	-22958.78	5.66	14.10	0.00	-26333.24	4.10	1.79	0.37
	6	5.71	14.16	2.57	P1	5.63	14.55	0.15	-23679.30	5.67	14.10	0.00	-26838.94	3.73	1.58	0.15
	7	5.61	14.12	3.40	P3 121											
	8	5.70	14.08	3.21	P1											
	9	5.60	14.08	2.98	Cm	5.70	14.57	0.58	-22650.38	5.66	14.10	0.00	-26563.87	5.03	1.79	0.28
	10	5.77	13.91	3.16	Cm											
	11	5.75	14.14	4.21	P-1	5.64	14.76	0.83	-22447.66	5.79	14.50	3.09	-25532.18	3.60	0.52	3.61
	12	5.45	14.09	3.83	P-1											
	13	5.63	14.15	4.00	C2/m	5.67	14.55	0.14	-22551.40	5.76	14.31	1.91	-25518.82	3.39	0.00	2.07
	14	5.70	13.92	3.85	Pm											
	15	5.63	14.00	3.16	P-1											
	16	5.72	13.90	2.65	P1											
	17	5.67	14.13	3.78	P2/m	5.64	14.54	0.55	-22805.45	5.88	14.47	3.08	-25637.93	3.16	0.51	3.32
	18	5.47	14.06	3.97	P-1											
	19	5.68	14.07	2.89	P1											
	20	5.50	14.01	2.74	Cm											
	21	5.69	13.90	2.83	C2/m	5.64	14.60	0.14	-23437.53	5.66	14.08	0.00	-26664.41	3.84	1.79	0.16
	22	5.65	13.93	4.26	C2/m	5.75	14.35	0.53	-22268.21	5.82	14.31	0.00	-25521.16	3.89	0.78	0.23
	23	5.64	13.96	2.84	P-1	5.63	14.52	0.34	-23504.14	5.67	14.09	0.00	-26657.53	3.71	1.58	0.04
	24	5.45	14.18	3.15	P2/m	5.64	14.56	0.46	-23258.24	5.66	14.11	0.00	-26455.50	3.79	1.79	0.16
	25	5.54	13.93	3.54	P-1											
	26	5.62	14.06	3.96	P1	5.68	14.58	1.03	-22611.16	5.80	14.53	3.08	-25634.81	3.49	1.51	3.80
	27	5.66	14.18	3.90	Pm	5.65	14.42	0.13	-22611.37	5.76	14.31	1.91	-25568.20	3.38	0.00	2.08
	28	5.60	14.23	5.05	P1											
	29	5.42	14.13	3.87	P-1											
	30	5.44	14.07	3.90	P1											

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
5	1	5.54	14.13	3.79	P-1											
	2	5.68	14.11	3.74	Cm	5.65	14.58	0.61	-22772.21	5.89	14.47	3.07	-25652.76	3.24	0.51	3.38
	3	5.74	14.08	3.39	Cm	5.63	14.63	0.61	-23050.79	5.77	14.30	1.87	-25815.56	3.04	0.00	2.17
	4	5.63	13.97	3.99	Cm	5.66	14.51	0.50	-22610.23	5.88	14.47	3.08	-25560.47	3.36	0.52	3.29
	5	5.59	14.07	3.83	Cm	5.64	14.54	0.58	-22766.58	5.66	14.11	0.00	-26017.16	3.88	0.00	0.28
	6	5.60	13.93	3.28	P1	5.62	14.49	0.52	-23149.57	5.66	14.09	0.00	-26367.29	3.83	1.79	0.22
	7	5.44	14.10	3.33	P1											
	8	5.45	14.18	3.89	P1											
	9	5.63	14.00	3.29	P-1											
	10	5.45	14.15	4.18	Cm											
	11	5.62	14.15	3.93	P1	5.66	14.59	0.67	-22638.61	5.80	14.29	1.28	-25705.75	3.57	0.35	1.65
	12	5.56	14.01	4.25	P3 121											
	13	5.74	13.97	4.16	P-1	5.66	14.60	0.72	-22321.39	5.85	14.50	3.09	-25515.19	3.78	0.72	3.50
	14	5.61	13.96	3.34	P-1											
	15	5.56	14.10	3.81	P-1	5.64	14.50	0.38	-22821.04	5.66	14.13	0.00	-26026.91	3.81	2.00	0.08
	16	5.65	14.05	3.16	P-1											
	17	5.63	14.10	3.83	Pm	5.64	14.40	0.39	-22698.18	5.80	14.28	1.27	-25758.50	3.55	0.35	1.36
	18	5.62	14.06	3.68	P1											
	19	5.61	14.08	3.94	Cm	5.63	14.55	0.77	-22641.65	5.80	14.28	1.28	-25698.60	3.55	0.30	1.74
	20	5.67	14.00	3.16	P-1	5.63	14.55	0.18	-23263.47	5.66	14.09	0.00	-26448.64	3.77	2.00	0.12
	21	5.48	14.07	3.78	Cm											
	22	5.70	14.02	4.58	Cm	5.71	14.61	1.07	-22005.85	5.83	14.57	3.05	-24979.15	3.40	1.10	3.87
	23	5.60	13.93	4.26	C2/m	5.69	14.29	0.64	-22322.60	5.72	14.24	1.27	-26438.40	3.84	0.00	1.61
	24	5.76	13.90	3.15	P1											
	25	5.68	14.11	3.20	Cm											
	26	5.50	14.01	4.10	P1											
	27	5.60	13.99	3.16	P1	5.63	14.51	0.42	-23236.98	5.66	14.08	0.00	-26445.62	3.81	1.79	0.12
	28	5.67	13.97	3.52	Cm											
	29	5.58	14.08	3.63	P-1											
	30	5.60	14.12	3.50	Pm											

Table S2 Continued

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
6	1	5.63	14.00	3.16	P-1											
	2	5.44	14.09	3.84	P1											
	3	5.64	14.05	4.19	P-1	5.67	14.62	0.94	-22435.51	5.76	14.30	1.93	-25430.56	3.44	0.30	2.57
	4	5.69	14.06	3.50	P1											
	5	5.62	13.93	3.20	P-1											
	6	5.62	14.08	4.12	P1	5.65	14.56	0.79	-22513.20	5.88	14.47	3.09	-25513.34	3.45	0.72	3.57
	7	5.72	13.92	3.43	P1	5.63	14.69	0.39	-23002.99	5.78	14.51	2.59	-25520.48	2.62	0.98	2.68
	8	5.44	14.11	3.07	P1											
	9	5.51	14.11	3.76	Cm											
	10	5.57	14.07	3.06	Cm	5.63	14.50	0.49	-23289.90	5.66	14.10	0.00	-26510.04	3.83	1.79	0.19
	11	5.42	14.12	4.00	P2/m											
	12	5.61	13.95	3.05	P1	5.62	14.47	0.09	-23293.79	5.66	14.08	0.00	-26517.43	3.84	1.58	0.21
	13	5.60	14.09	3.95	P1	5.63	14.55	0.40	-22660.58	5.88	14.46	3.08	-25574.90	3.30	0.72	3.18
	14	5.64	14.13	4.17	Cm	5.65	14.63	0.54	-22484.05	5.80	14.51	3.08	-25553.35	3.57	0.51	3.33
	15	5.71	14.05	3.12	Cm	5.64	14.51	0.38	-23259.92	5.66	14.09	0.00	-26476.36	3.82	1.79	0.08
	16	5.74	13.91	3.21	Cm	5.65	14.50	0.27	-23197.05	5.69	14.13	0.47	-26085.06	3.26	0.00	0.50
	17	5.66	14.09	3.89	P1											
	18	5.50	14.02	3.39	Cm											
	19	5.55	14.07	3.73	Cm											
	20	5.59	14.12	3.51	P-1											
	21	5.78	14.14	4.21	P-1	5.67	14.62	1.14	-22298.18	5.80	14.51	3.09	-25534.44	3.86	0.72	3.93
	22	5.52	14.08	3.71	Cm											
	23	5.60	13.95	3.05	P1	5.63	14.49	0.51	-203290.34	5.66	14.08	0.00	-26504.98	3.82	1.58	0.21
	24	5.62	14.15	5.01	P1	5.68	14.62	0.98	-21887.68	5.84	14.57	3.12	-25206.22	4.00	0.51	3.79
	25	5.60	14.16	5.05	P2/m	5.71	14.71	1.00	-21770.24	5.79	14.51	3.12	-25252.22	4.28	0.92	3.81
	26	5.67	14.08	3.29	Cm	5.64	14.64	0.45	-23112.62	5.66	14.11	0.00	-26364.98	3.89	1.79	0.15
	27	5.60	14.07	3.28	P-1											
	28	5.68	14.03	3.91	P3_221	5.69	14.59	0.72	-22657.30	5.76	14.30	1.91	-25563.11	3.29	0.00	2.32
	29	5.63	14.21	4.26	Cm	5.70	14.68	0.80	-22429.60	5.88	14.47	3.09	-25463.41	3.51	0.93	3.59
	30	5.56	14.01	4.02	P-1											

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
7	1	5.58	14.11	3.24	P3_221											
	2	5.67	14.15	3.71	P1	5.63	14.54	0.69	-22789.46	5.88	14.47	3.07	-25663.94	3.23	0.52	3.46
	3	5.63	14.02	3.98	P1	5.69	14.57	0.72	-22526.44	5.76	14.30	1.91	-25526.22	3.45	0.00	2.34
	4	5.52	14.04	3.28	P1											
	5	5.65	14.05	3.91	P-1	5.63	14.53	0.64	-22687.04	5.88	14.47	3.08	-25589.87	3.28	0.72	3.41
	6	5.54	14.17	3.46	P-1											
	7	5.60	13.95	3.05	P1	5.64	14.50	0.51	-23297.21	5.66	14.08	0.00	-26516.98	3.83	1.58	0.21
	8	5.59	14.14	3.95	P1	5.65	14.57	0.49	-22631.73	5.72	14.20	0.64	-25806.20	3.75	0.49	0.82
	9	5.56	14.08	3.06	Cm	5.63	14.51	0.51	-23300.86	5.66	14.11	0.00	-26509.51	3.81	1.79	0.21
	10	5.59	14.08	3.73	P1											
	11	5.66	14.11	4.39	Cm											
	12	5.46	14.15	3.38	Cm											
	13	5.73	14.00	4.14	Cm	5.66	14.56	0.51	-22478.18	5.80	14.58	3.06	-25383.90	3.29	0.74	3.27
	14	5.59	14.03	3.59	Cm	5.63	14.52	0.16	-22915.31	5.66	14.10	0.00	-26168.20	3.89	1.79	0.14
	15	5.65	14.09	3.82	Cm	5.65	14.61	0.58	-22749.98	5.94	14.36	1.92	-25692.66	3.35	0.35	2.19
	16	5.59	14.05	3.08	P-1	5.64	14.49	0.54	-23314.41	5.66	14.10	0.00	-26497.88	3.77	1.58	0.24
	17	5.60	13.93	4.26	C2/m	5.69	14.29	0.64	-22322.60	5.72	14.24	1.27	-46601.72	3.50	0.00	1.61
	18	5.62	14.09	4.36	P-1	5.66	14.66	1.01	-22325.41	5.76	14.31	1.95	-25351.99	3.50	0.00	2.65
	19	5.52	14.07	3.81	P1											
	20	5.64	14.15	3.82	P1											
	21	5.59	14.07	3.06	Cm	5.64	14.51	0.32	-23293.94	5.66	14.10	0.00	-26511.08	3.82	1.79	0.02
	22	5.60	14.10	3.95	P1											
	23	5.49	14.08	3.71	Cm											
	24	5.52	14.07	3.71	Cm											
	25	5.45	14.18	3.89	P1											
	26	5.74	14.08	4.04	Cm	5.65	14.54	0.85	-22541.04	5.85	14.59	3.08	-25544.82	3.46	0.00	3.63
	27	5.49	14.12	3.82	P-1											
	28	5.71	13.99	4.12	Cm	5.67	14.66	0.66	-22477.60	5.76	14.31	1.93	-25467.01	3.43	0.00	2.29
	29	5.74	14.01	3.81	P-1	5.67	14.59	0.84	-22770.32	5.76	14.30	1.90	-25613.47	3.18	0.00	2.44
	30	5.61	13.96	3.50	Cm											

Table S2 Continued

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
8	1	5.63	13.96	3.47	P-1											
	2	5.63	13.97	3.50	P1											
	3	5.60	14.02	4.33	Cm	5.64	14.62	0.41	-22428.88	5.75	14.30	1.94	-25362.38	3.33	0.00	2.06
	4	5.60	14.09	4.34	P3_221	5.65	14.69	0.79	-22372.88	5.75	14.31	1.94	-25358.94	3.43	0.00	2.43
	5	5.71	14.08	3.80	Cm	5.71	14.67	0.89	-22707.34	5.80	14.54	3.07	-25694.50	3.43	0.51	3.66
	6	5.60	14.07	3.53	Cm											
	7	5.64	14.15	4.54	P1											
	8	5.66	14.07	3.77	P1	5.67	14.55	0.55	-22745.99	5.80	14.67	3.01	-25226.51	2.55	1.63	3.27
	9	5.62	14.06	3.85	P-1											
	10	5.58	13.96	3.32	P1											
	11	5.52	14.07	3.78	P1											
	12	5.58	13.99	3.09	P1	5.63	14.51	0.16	-23272.49	5.66	14.08	0.00	-26490.18	3.83	1.79	0.14
	13	5.60	13.95	3.15	Cm	5.63	14.51	0.58	-23221.02	5.66	14.08	0.00	-26451.82	3.85	1.79	0.28
	14	5.60	14.09	3.32	P-1											
	15	5.60	14.16	4.66	Cm	5.66	14.60	0.72	-22146.90	5.88	14.47	3.11	-25323.62	3.76	0.93	3.53
	16	5.57	14.04	3.16	P1	5.63	14.49	0.34	-23221.59	5.66	14.10	0.00	-26444.64	3.84	1.79	0.04
	17	5.58	14.08	3.58	P1											
	18	5.62	14.15	4.29	P3_121	5.66	14.68	0.90	-22347.75	5.76	14.31	1.94	-25384.69	3.51	0.00	2.54
	19	5.60	14.02	3.18	Cm	5.63	14.49	0.16	-23227.82	5.66	14.09	0.00	-26432.94	3.80	1.79	0.14
	20	5.60	14.03	3.86	P1	5.63	14.53	0.59	-22733.88	5.66	14.11	0.00	-25996.60	3.90	2.21	0.29
	21	5.60	14.07	3.23	Cm											
	22	5.66	14.02	5.29	Cm	5.67	14.63	0.69	-21681.46	5.85	14.42	0.00	-25090.10	4.16	0.00	0.39
	23	5.61	13.95	3.05	P1	5.67	14.51	0.73	-23243.20	5.66	14.08	0.00	-26517.43	3.92	1.58	0.43
	24	5.59	14.03	3.59	Cm	5.63	14.55	0.55	-22928.36	5.66	14.10	0.00	-26168.20	3.86	1.79	0.25
	25	5.71	14.00	3.12	Cm											
	26	5.52	14.03	3.81	P1											
	27	5.71	14.05	2.70	Cm	5.64	14.52	0.33	-23576.43	5.67	14.09	0.00	-26752.02	3.75	1.79	0.03
	28	5.59	14.06	3.03	P1	5.63	14.52	0.14	-23324.79	5.66	14.10	0.00	-26530.58	3.81	1.79	0.16
	29	5.59	14.04	3.59	Cm											
	30	5.59	14.02	3.03	Cm	5.63	14.51	0.51	-23326.06	5.66	14.09	0.00	-26530.26	3.80	1.79	0.21

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
9	1	5.60	14.04	3.56	Cm											
	2	5.59	14.08	3.13	P-1	5.62	14.52	0.45	-23269.33	5.66	14.10	0.00	-26465.58	3.79	1.79	0.15
	3	5.66	14.05	3.92	P1	5.65	14.60	0.07	-22693.25	5.88	14.47	3.08	-25586.20	3.26	0.72	3.31
	4	5.69	14.00	4.12	P-3m1											
	5	5.59	14.13	3.43	Cm											
	6	5.73	14.00	4.14	Cm	5.65	14.56	0.46	-22454.99	5.80	14.58	3.06	-25383.90	3.33	0.71	3.21
	7	5.56	14.10	3.95	P-1	5.64	14.51	0.39	-22726.52	5.82	14.36	2.16	-25441.02	2.96	1.91	2.24
	8	5.61	14.09	3.69	P1											
	9	5.59	14.09	3.90	P1											
	10	5.61	14.03	3.58	Cm	5.63	14.51	0.22	-22938.60	5.66	14.10	0.00	-26175.55	3.86	2.00	0.08
	11	5.59	14.07	3.56	C2/m											
	12	5.42	14.13	4.08	Cm	5.65	14.61	0.66	-22540.38	5.82	14.36	2.17	-25381.08	3.17	2.13	2.53
	13	5.62	14.10	3.92	P1											
	14	5.61	14.11	4.06	Cm	5.63	14.56	0.59	-22615.45	5.76	14.31	1.92	-25488.54	3.23	0.00	2.21
	15	5.60	14.11	3.70	P1											
	16	5.60	14.08	4.40	Cm	5.67	14.42	0.07	-22272.97	5.88	14.46	3.10	-25413.70	3.69	0.93	3.32
	17	5.61	14.02	3.64	P1											
	18	5.66	14.07	3.77	Cm	5.67	14.55	0.54	-22721.90	5.80	14.67	3.01	-25226.51	2.59	1.63	3.26
	19	5.73	14.08	3.80	Cm	5.70	14.62	0.92	-22636.21	5.76	14.31	1.90	-25618.50	3.42	0.00	2.52
	20	5.59	14.03	3.59	Pm	5.64	14.36	0.69	-22793.44	5.66	14.10	0.00	-26168.20	4.10	1.79	0.39
	21	5.71	14.08	3.80	P1	5.67	14.67	0.47	-22730.55	5.80	14.53	3.07	-25695.98	3.39	0.31	3.24
	22	5.59	14.03	3.59	Cm	5.63	14.52	0.16	-22915.29	5.66	14.10	0.00	-26168.20	3.89	1.79	0.14
	23	5.62	14.17	4.36	P-1	5.65	14.56	1.00	-22324.09	5.88	14.47	3.10	-25427.83	3.63	0.72	3.80
	24	5.66	14.10	3.29	Cm	5.63	14.60	0.30	-23144.53	5.66	14.10	0.00	-26365.13	3.83	2.00	0.00
	25	5.59	14.03	4.53	Cm											
	26	5.68	14.12	4.42	P1	5.64	14.70	0.59	-22368.91	5.82	14.48	3.10	-25426.20	3.55	0.72	3.39
	27	5.65	14.15	4.29	P3 121											
	28	5.60	14.07	3.06	P1	5.64	14.60	0.33	-23322.30	5.66	14.10	0.00	-26511.52	3.78	1.79	0.03
	29	5.58	14.07	3.22	Cm	5.63	14.52	0.34	-23169.87	5.66	14.11	0.00	-26406.43	3.86	1.79	0.04
	30	5.66	14.07	3.77	P1	5.63	14.55	0.58	-22781.99	5.80	14.66	3.01	-25226.52	2.49	1.64	3.30

Table S2 Continued

Gen.	No.	Decision Variable				Calculated								Object Function		
						Li _{0.5} CO ₂				LiCoO ₂						
		a	c	U	Space G.	a	c	μ _{average}	Total E.	a	c	μ _{average}	Total E.	E ^{redox}	E _b	Mag. Dev.
10	1	5.66	14.13	4.41	P1	5.63	14.63	0.16	-22311.57	5.76	14.32	1.95	-25333.38	3.49	0.00	2.10
	2	5.62	14.18	5.01	P1	5.68	14.72	0.84	-21936.88	5.80	14.52	2.62	-24802.28	3.22	2.36	3.20
	3	5.59	14.02	3.18	Cm	5.63	14.67	0.32	-23218.95	5.66	14.09	0.00	-26432.53	3.82	1.79	0.02
	4	5.60	14.10	4.35	Cm	5.66	14.63	0.84	-22303.42	5.75	14.31	1.95	-25354.54	3.54	0.00	2.48
	5	5.63	14.11	3.61	P1	5.66	14.57	0.39	-22892.30	5.66	14.12	0.00	-26157.89	3.91	2.00	0.09
	6	5.60	14.03	3.82	P1											
	7	5.62	14.13	4.19	P-1	5.63	14.80	0.69	-22501.06	5.82	14.53	3.09	-25535.86	3.51	0.52	3.47
	8	5.65	14.11	3.97	C2/m											
	9	5.56	14.10	3.81	P3 121	5.62	14.50	0.41	-22798.62	5.66	14.13	0.00	-26026.91	3.84	2.21	0.11
	10	5.64	14.15	4.31	P1	5.63	14.57	0.21	-22455.29	5.76	14.32	1.94	-25377.23	3.31	0.00	2.04
	11	5.62	14.14	3.71	Cm	5.62	14.52	0.26	-22790.22	5.66	14.13	0.00	-26093.83	3.97	1.97	0.04
	12	5.58	14.03	3.49	P1	5.64	14.49	0.28	-22979.67	5.66	14.10	0.00	-26231.76	3.89	1.97	0.02
	13	5.62	14.08	4.07	Cm	5.67	14.70	0.31	-22541.02	5.94	14.36	1.93	-25575.46	3.51	0.15	1.95
	14	5.6	14.04	3.59	P-3m1	5.63	14.29	0.53	-22838.40	5.66	14.10	0.00	-26168.74	4.02	1.79	0.23
	15	5.64	14.02	4.42	Cm											
	16	5.62	14.02	3.55	Cm											
	17	5.63	14.06	3.94	Cm	5.63	14.52	0.40	-22681.75	5.76	14.31	1.91	-25545.44	3.21	0.00	2.01
	18	5.64	14.12	4.27	Cm	5.66	14.56	0.59	-22432.24	5.90	14.43	2.72	-25455.95			
	19	5.42	14.19	4.02	P3 221	5.64	14.55	0.65	-22642.15	5.65	14.13	0.00	-25884.07	3.87	0.00	0.35
	20	5.57	14.16	4.66	Cm	5.66	14.63	0.50	-22123.82	5.75	14.31	1.98	-25213.84	3.61	0.00	2.18
	21	5.59	14.03	3.59	Pm	5.64	14.36	0.69	-22793.45	5.66	14.10	0.00	-26168.20	4.10	1.79	0.39
	22	5.59	14.08	2.94	P-1	5.63	14.71	0.35	-23435.54	5.66	14.10	0.00	-26589.66	3.72	1.79	0.05
	23	5.45	14.18	3.15	P1	5.64	14.61	0.56	-23186.17	5.66	14.10	0.00	-26455.50	3.92	1.78	0.26
	24	5.61	14.03	3.45	P1	5.64	14.55	0.42	-23002.00	5.66	14.10	0.00	-26259.00	3.89	1.98	0.12
	25	5.59	14.13	3.43	P1											
	26	5.59	14.12	3.43	Cm											
	27	5.61	13.95	3.01	Cm	5.63	14.49	0.33	-23338.54	5.66	14.10	0.00	-26546.86	3.81	1.79	0.03
	28	5.64	14.15	4.61	P1											
	29	5.60	14.09	4.34	P3 221	5.62	14.74	0.89	-22379.74	5.75	14.31	1.95	-25358.92	3.41	0.00	2.53
	30	5.61	14.10	4.34	P1	5.66	14.52	0.51	-22343.02	5.76	14.31	1.94	-25360.16	3.48	0.00	2.15