Supplementary Information

Efficient Preparation of Battery-Grade Li_2CO_3 from Spent Battery Leachate via Integrated Solvent Extraction and Direct Precipitation

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Table S1. The content of major elements in the raw material solution (mg/L)

Element	Ca	Co	Li	Na	Mg	Mn
Content	371.49	36.71	2485.89	20904.3	202.94	30.92
Element	Ni	B	F^-	Cl^-	SO_4^{2-}	CO_3^{2-}
Content	139.8	25.31	84.79	604.34	50187.9	3066.73

Table S2. Separation coefficients for $\beta_{Me/Li}$ (Me = Ca, Co, Mg, Mn and Ni)

Equilibrium pH	$\beta_{Ca/Li}$	$\beta_{Co/Li}$	$\beta_{Mg/Li}$	$\beta_{Mn/Li}$	$\beta_{Ni/Li}$
6.50	560.78	1748.85	252.90	12992.02	18.99
6.70	2063.53	2516.59	427.95	25428.02	50.33
7.00	1420.04	2127.98	367.50	20913.97	73.96
7.40	900.96	1356.64	302.09	10917.26	76.07

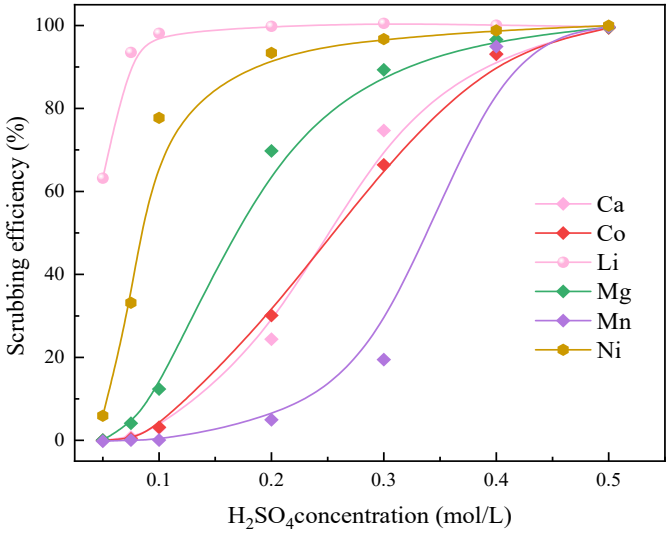

Fig.S1. Effect of H_2SO_4 concentration on the scrubbing efficiency of Ca, Co, Li, Mg, Mn, and Ni (O/A ratio: 6:1, t: 10 min, T: 20℃)

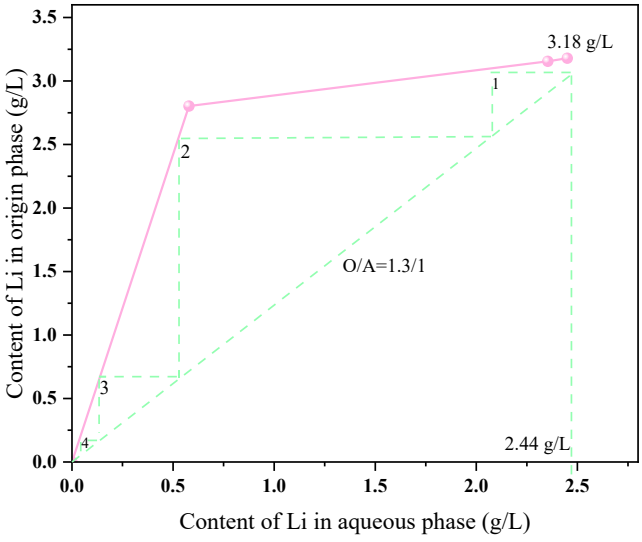

Fig. S2. McCabe-Thiele diagram for Li extraction

Table S3. Experimental results of Three-stage countercurrent extraction

Row	Raffinate (mg/L)						Extraction efficiency (%)						pHe
	Ca	Co	Li	Mg	Mn	Ni	Ca	Co	Li	Mg	Mn	Ni	
R6	≤0.5	0.84	2394.81	≤0.5	≤0.5	0.63	99.6	99.4	3.66	99.9	99.9	99.5	7.08
R7	≤0.5	0.65	2416.63	≤0.5	≤0.5	0.58	99.9	99.6	2.77	99.9	99.9	99.6	7.06
R8	≤0.5	≤0.5	2430.00	≤0.5	≤0.5	≤0.5	99.9	99.8	2.21	99.9	99.9	99.9	7.01

Table S4. Experimental results of multi-stage simulation experiment

Process		Metal concentration /(mg/L)					
		Ca	Co	Li	Mg	Mn	Ni
Extraction	raffinate	＜0.5	＜0.5	2430.01	＜0.5	＜0.5	＜0.5
	loaded organic phase	371.13	36.71	86.84	202.76	30.91	139.72
Scrubbing	scrubbing solution	14.07	0.32	497.32	28.77	0.20	276.29
	organic phase after scrubbing	368.78	36.66	3.95	197.97	30.88	93.67
Stripping	stripping solution	2212.27	219.85	23.70	1186.98	185.10	561.62

Table S5. The content of metal and non-metal ions (mg/L)

Element	Ca	Co	Li	Na	Mg	Mn	Ni	B	F^-	Cl^-	SO_4^{2-}	CO_3^{2-}
Content	≤0.5	≤0.5	2430	42476	≤0.5	≤0.5	≤0.5	21.16	70.55	529.98	40150.21	2396.01

Table S6. Experimental results of four-stage countercurrent extraction

Row	Raffinate (mg/L)		Extraction efficiency (%)	
	Li	Na	Li	Na
8	0.82	47688.99	99.9	1.33
9	0.73	47426.90	99.9	1.40
10	≤0.5	47352.89	>99.9	1.40

Table S7. Experimental results of five-stage countercurrent scrubbing

Row	Scrubbing solution (mg/L)					Scrubbing efficiency (%)				
	Li	Na	B	F^-	Cl^-	Li	Na	B	F^-	Cl^-
10	2804.51	6290.32	1.83	5.85	38.78	4.21	>99.9	>99.9	>99.9	>99.9
11	2821.79	6141.08	1.81	5.93	39.47	4.66	>99.9	>99.9	>99.9	>99.9
12	2867.69	6291.57	1.84	5.92	38.55	4.85	>99.9	>99.9	>99.9	>99.9

Table S8. Experimental results of two-stage countercurrent stripping

Row	Stripping solution (mg/L)		Stripping efficiency (%)	
	Li	Na	Li	Na
4	31963.44	42.29	>99.9	>99.9
5	32096.87	47.45	>99.9	>99.9
6	31871.09	48.02	>99.9	>99.9

Table S9. Chemical composition in the stripping solution (mg/L)

Element	Ca	Co	Li	Na	Mg	Mn	Ni	B	F^-	Cl^-	SO_4^{2-}	CO_3^{2-}
Sample-1	≤0.5	≤0.5	31962.49	419.27	≤0.5	≤0.5	≤0.5	≤0.5	≤0.5	≤0.5	180224.78	≤0.5
Sample-2	≤0.5	≤0.5	32099.01	406.59	≤0.5	≤0.5	≤0.5	≤0.5	≤0.5	≤0.5	180477.13	≤0.5
Sample-3	≤0.5	≤0.5	31871.98	418.05	≤0.5	≤0.5	≤0.5	≤0.5	≤0.5	≤0.5	180393.08	≤0.5

Table S10. Comparison of the synthesized Li_2CO_3 with the battery-grade standard (YS/T 582-2023).

YS/T 582-2023 Mass fraction (%)	Li_2CO_3-D1	Li_2CO_3-D2	Li_2CO_3-D3	Li_2CO_3 product
Li_2CO_3	≥99.5%	≥99.5%	≥99.5%	99.7%
Na	≤0.005	≤0.020	≤0.025	≤0.020
Mg	≤0.001	≤0.005	≤0.008	≤0.005
Ca	≤0.002	≤0.005	≤0.008	≤0.005
K	≤0.001	≤0.005	≤0.010	≤0.005
Fe	≤0.0005	≤0.0010	≤0.0020	≤0.020
Zn	≤0.0001	≤0.0003	≤0.0005	≤0.0001
Cu	≤0.0001	≤0.0003	≤0.0005	≤0.0001
Pb	≤0.0001	≤0.0003	≤0.0005	≤0.0001
Si	≤0.002	≤0.003	≤0.005	≤0.002
Al	≤0.0005	≤0.0010	≤0.0020	≤0.0005
Mn	≤0.0001	≤0.0003	≤0.0005	≤0.0001
Ni	≤0.0001	≤0.0003	≤0.0005	≤0.0001
B	≤0.001	≤0.003	≤0.005	≤0.001
SO_4^{2-}	≤0.04	≤0.07	≤0.08	≤0.04
Cl^-	≤0.002	≤0.003	≤0.005	≤0.003

Table S11. Experimental conditions for the continuous extraction, scrubbing, stripping, and washing stages

	Stage	T (°C)	Time (min)	O/A	Regent	Concentration
Extraction	4	25	5	1.5/1	Feeds/ NaOH	/
Scurbbing	5	25	10	10/1	H_2SO_4	0.5 mol/L
Stripping	2	25	10	10/1	H_2SO_4	2.0 mol/L
Washing	2	25	10	12/1	H_2O	/

Table S12. Experimental data of the continuous extraction, scrubbing, and stripping

Time (h)	Extraction								Scrubbing				Stripping			
	Flow (mL/min)			Raffinate				H_2SO_4	Scrubbing solution			H_2SO_4	Stripping solution			
	Feed	Organic	NaOH	Li (mg/L)	Na (g/L)	pH	TOC	(mL/min)	Li (g/L)	Na (g/L)	pH	(mL/min)	Li (g/L)	Na (mg/L)	pH	TOC
100	9.4	14.1	0.3	300.39	36.76	12.98	53.15	1.4	2.28	4.32	12.65	1.4	24.98	73.54	2.54	6.34
120	9.4	14.1	0.3	280.87	36.82	12.99	56.31	1.4	2.35	4.20	12.41	1.4	24.08	77.98	2.62	6.84
140	9.4	14.1	0.3	160.06	38.01	13.02	53.12	1.4	2.19	4.28	12.53	1.4	25.88	80.01	2.41	6.64
160	9.4	14.1	0.3	146.54	38.01	13.02	58.64	1.4	2.41	4.35	12.38	1.4	25.01	76.14	2.43	6.33
180	9.4	14.1	0.3	113.61	38.26	13.11	55.46	1.4	2.24	4.23	12.81	1.4	26.66	69.22	2.43	6.48
200	9.4	14.1	0.3	100.12	38.11	13.01	53.55	1.4	2.31	4.18	12.46	1.4	26.27	76.35	2.39	6.86
220	9.4	14.1	0.3	83.11	38.88	12.89	56.46	1.4	2.37	4.40	12.59	1.4	26.11	73.99	2.46	6.64
240	9.4	14.1	0.3	66.12	37.01	12.89	54.15	1.4	2.22	4.37	12.33	1.4	27.21	61.09	2.41	6.34
260	9.4	14.1	0.3	61.03	37.66	13.01	57.13	1.4	2.39	4.31	12.61	1.4	26.89	66.01	2.40	6.39
280	9.4	14.1	0.3	52.55	38.11	13.11	59.11	1.4	2.26	4.42	12.49	1.4	26.01	50.1	2.66	6.48
300	9.4	14.1	0.3	42.09	36.98	12.91	57.21	1.4	2.33	4.29	12.56	1.4	26.03	60.98	2.54	6.39
320	9.4	14.1	0.3	35.11	37.35	13.13	53.64	1.4	2.20	4.38	12.68	1.4	26.09	71.25	2.31	6.34

340	9.3	14.1	0.3	11.78	38.22	13.01	55.94	1.4	2.40	4.39	12.44	1.4	26.55	84.12	2.55	6.32
360	9.3	14.1	0.3	4.01	40.55	13.01	52.45	1.4	2.38	4.24	12.37	1.4	28.34	97.11	2.45	6.42
380	9.3	14.1	0.3	6.98	40.01	12.98	54.38	1.4	2.32	4.27	12.63	1.4	27.06	72.57	2.54	6.45
400	9.3	14.1	0.3	5.01	40.21	13.19	51.85	1.4	2.35	4.41	12.44	1.4	27.87	83.14	2.77	6.35
420	9.3	14.1	0.3	5.21	40.22	12.95	49.71	1.4	2.37	4.35	12.37	1.4	28.09	80.14	2.77	6.45
440	9.3	14.1	0.3	5.95	39.01	12.98	46.78	1.4	2.37	4.32	12.63	1.4	28.20	88.13	2.70	6.82
460	9.3	14.1	0.3	5.36	38.79	12.20	47.64	1.4	2.38	4.33	12.50	1.4	29.03	80.32	2.66	6.34
480	9.3	14.1	0.3	10.98	41.28	12.98	45.46	1.4	2.38	4.33	12.60	1.4	28.82	79.89	2.65	6.45
500	9.3	14.1	0.3	8.01	40.11	12.84	43.68	1.4	2.38	4.35	12.48	1.4	28.03	77.11	2.65	6.13
520	9.3	14.1	0.3	6.01	39.49	12.87	41.45	1.4	2.38	4.37	12.66	1.4	28.13	62.11	2.76	6.64
540	9.3	14.1	0.3	4.02	40.70	12.76	42.63	1.4	2.36	4.37	12.39	1.4	27.72	53.01	2.76	6.31
560	9.3	14.1	0.3	3.98	42.16	12.56	41.57	1.4	2.38	4.32	12.57	1.4	27.12	58.23	2.70	6.29
580	9.3	14.1	0.3	2.03	40.99	12.67	41.17	1.4	2.38	4.36	12.45	1.4	27.19	48.21	2.70	6.09
600	9.3	14.1	0.3	1.04	40.14	12.97	41.36	1.4	2.38	4.39	12.52	1.4	28.23	41.32	2.65	6.41
620	9.3	14.1	0.3	≤0.5	41.11	12.45	40.45	1.4	2.37	4.39	12.58	1.4	28.21	40.11	2.66	6.19
640	9.3	14.1	0.3	≤0.5	42.11	12.63	40.69	1.4	2.38	4.39	12.57	1.4	28.01	41.25	2.67	6.12
660	9.3	14.1	0.3	≤0.5	42.16	12.84	40.54	1.4	2.37	4.39	12.56	1.4	28.11	40.14	2.62	6.28
680	9.3	14.1	0.3	≤0.5	42.11	12.51	39.33	1.4	2.38	4.39	12.53	1.4	28.11	39.14	2.62	6.35
700	9.3	14.1	0.3	≤0.5	42.12	12.63	40.97	1.4	2.38	4.39	12.50	1.4	28.52	36.94	2.64	6.14
720	9.3	14.1	0.3	≤0.5	42.76	12.58	40.34	1.4	2.38	4.39	12.50	1.4	28.01	33.25	2.63	6.54

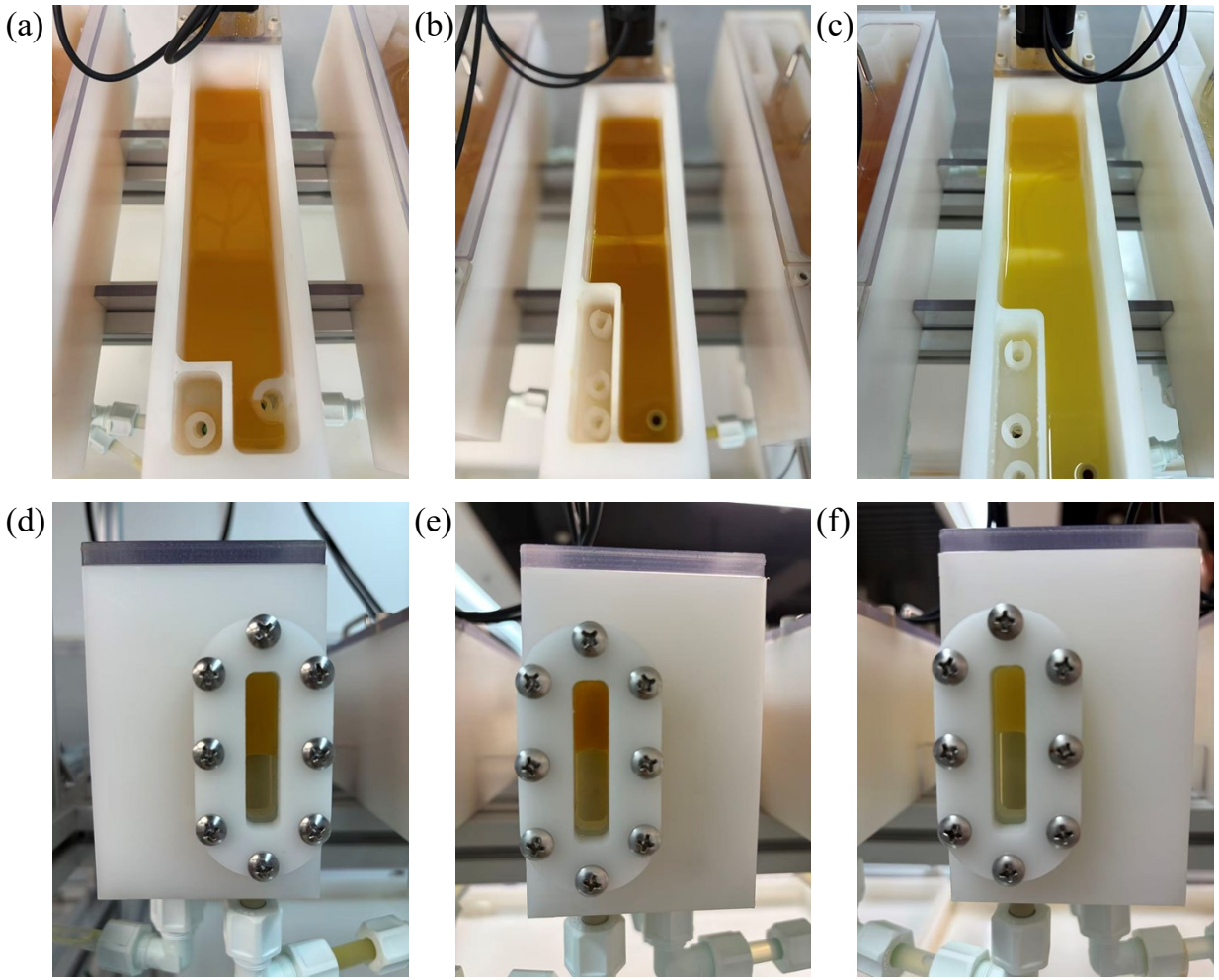

Fig.S3. Schematics of the mixed settlers for (a) extraction, (b) scrubbing, and (c) stripping stages; Phase interfaces observed during the (d) extraction, (e) scrubbing, and (f) stripping stages, respectively.

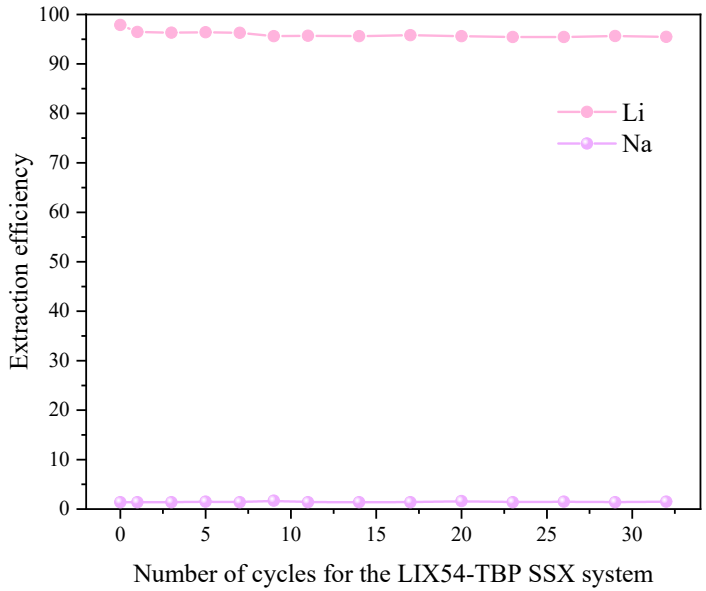

Fig.S4. Cycling extraction performance for the LIX54-TBP SSX system

Table S13. Cost accounting table (Exchange rate: RMB to USD and quotations of industrial raw materials are as of February, 2026)

	Items	Unit price	Impurity co-extraction cost		Li extraction cost		Li precipitation	
		$/t	t/t Li_2CO_3	$/t Li_2CO_3	t/t Li_2CO_3	$/t Li_2CO_3	t/t Li_2CO_3	$/t Li_2CO_3
Regents	NaOH (32%)	125.74	0.47	59.10	4.50	565.93	-	-
	H_2SO_4 (98%)	34.23	0.2	6.84	1.41	48.16	-	-
	D2EHPA	4881.45	2.7×10^{-3}	13.18	-	-	-	-
	LIX54/TBP	29288.70	-	-	3.6×10^{-3}	105.44	-	-
	Activated carbon	1117.69	-	-	0.01	11.18	-	-
	Activated carbon treatment	181.63	-	-	0.01	1.82	-	-
	Na_2CO_3	276.54	-	-	-	-	1.58	436.93
Cost				79.12		732.53		436.93
Products	Name	Unit price ($/t)	Cost($/t)	Yield (t)				Profit ($)
	Li_2CO_3	21000	1248.58	1				19751.42

Note: The cost accounting presented does not account for depreciation, energy consumption, or labor costs.