Low Reversible Capacity of Nitridated Titanium Electrical Terminals

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Table S1. Detailed composition of the raw materials used to machine the electrode terminals.

Label	Composition
St-304	C (max. 0.07%), Si (max. 1%), Mn (max. 2%), P (max. 0.045%), S (max. 0.03%), **Cr** (17.5–19.5%), **Ni** (8–10.5%), N (max. 0.1%), **Fe** (66.75–74.5) from DIN EN 10088-3
St-316L	C (max. 0.03%), Si (max. 1%), Mn (max. 2%), P (max. 0.045%), S (max. 0.03%), **Cr** (16.5–18.5%), **Mo** (2–2.5%), **Ni** (10–13%), N (max. 0.1%), **Fe** (62.8–71.5) from DIN EN 10088-3
St-304-old	Electrical terminal made of St-304 (see above) which was used over ca. one year.
Ti	Titanium grade 1.
Ti-NH_3	Thermally annealed titanium in an ammonia atmosphere.
Cu	Oxygen free copper.
FeNi	FeNi alloy steel with the following composition based on X-ray fluorescence measurements. Fe (63%), Ni (37%).
Coin cell	Coin cells based on a 2032 geometry (20 mm in diameter and 3.2 mm in thickness), acquired from MTI Corp. using stainless steel 304 as the case material.

Table S2. Detailed list of electrochemical cells and material. Duplicates are referred to as “a” and “b”.

Cell number	Electrode terminal	Description	Electrolyte	Raw data reference[3]
1	Coin cell/Cu_a	Coin cell with a 25 m thick copper foil as anode	LP71[1]	25164
2	Coin cell/Cu_b	Duplicate of cell 1	LP71	25165
3	Coin $cell_a$	Coin cell with lithium and separator only (cell 1 without copper)	LP71	25166
4	Coin $cell_b$	Duplicate of cell 4	LP71	25167
5	St-304-old_a	Terminal which was used over ca. 1 year	LP40[2]	21754
6	St-304-old_b	Duplicate of cell 5	LP40	21755
7	St-304_a	Terminal made of St-304	LP40	24490
8	St-304_b	Duplicate of 7	LP40	24491
9	St-$316L_a$	Terminal made of St-316L	LP40	24492
10	St-$316L_b$	Duplicate of 9	LP40	24493
11	$FeNi_a$	Terminal made of FeNi alloy	LP40	22792
12	$FeNi_b$	Duplicate of cell 11	LP40	22793
13	Cu_a	Oxygen-free copper	LP40	24494
14	Cu_b	Duplicate of cell 13	LP40	24495
15	Ti-NH_3-LP71	Titanium terminal thermally annealed in ammonia using LP71 electrolyte	LP40	24782
16	Ti_a	Titanium grade 1	LP40	23057
17	Ti_b	Duplicate of cell 16	LP40	23058
18	Ti-NH_{3a}	Titanium terminal thermally annealed in ammonia	LP40	23059
19	Ti-NH_{3b}	Duplicate of cell 19	LP40	23060
20	PEEK/St-304 (1 mm)	Terminal made in PEEK where a 1mm in diameter St-304 shaft was inserted	LP40	21966

[1] LP71 electrolyte composition: EC:DEC:DMC (1:1:1 vol.%) and 1M $LiPF_6$

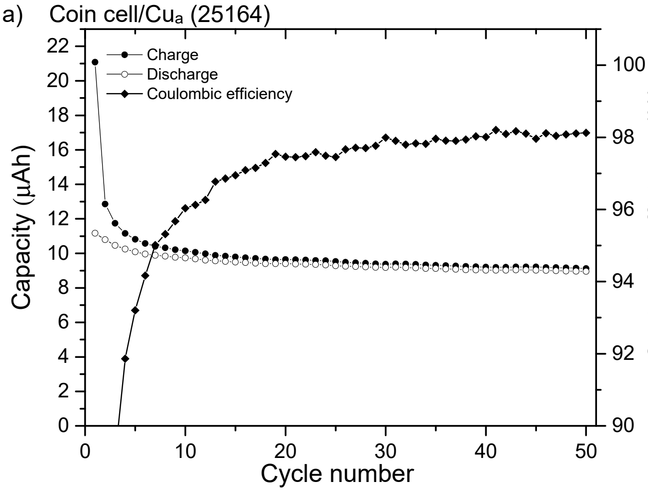
[2] LP40 electrolyte composition: EC:DEC (1:1 vol.%) and 1M $LiPF_6$.

Table S3. Initial and final specific discharge capacity of the selected electrode terminals, corresponding to Figure 2. The averaged and standard deviation values are calculated from the duplicate measurements. Similarly, the equivalent Si thickness in nm per geometric area is given (considering an equivalence value of 0.833 μAh nm^{-1} cm^{-1}).

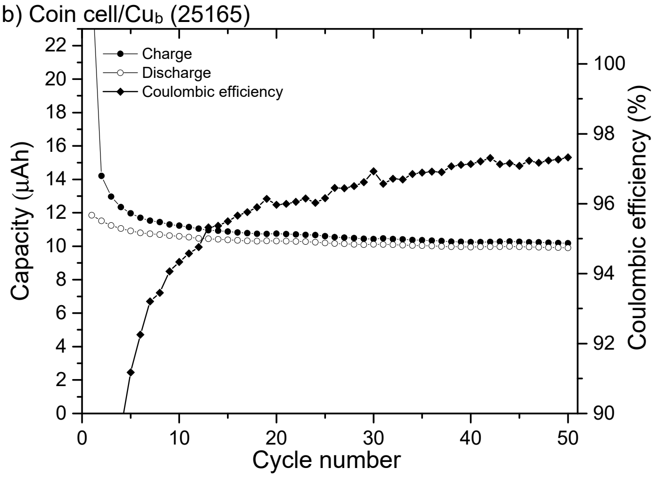
Materials	Discharge capacity (Ah)		Equivalent Si thickness (nm / $cm^2_{Geometric}$)	
	First cycle	50th cycle	First cycle	50th cycle
St-304	12.17±0.45	9.34±0.54	14.6±0.54	11.21±0.65
Coin cell	11.51±0.48	9.43±0.67	13.82±0.58	11.31±0.81
St-316L	10.56±0.33	7.96±0.61	12.68±0.39	9.56±0.73
Cu	8.14±0.94	5.28±1.03	9.77±1.13	6.33±1.23
Ti	1.99±0.30	1.10±0.13	2.39±0.36	1.32±0.15
TiN	0.79±0.19	0.60±0.20	0.95±0.22	0.72±0.24

Detailed electrochemical cycling

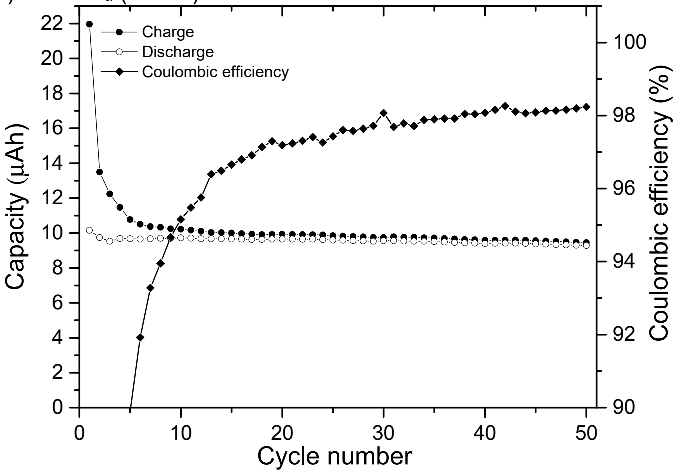
a) Coin cell/Cu_a (25164)



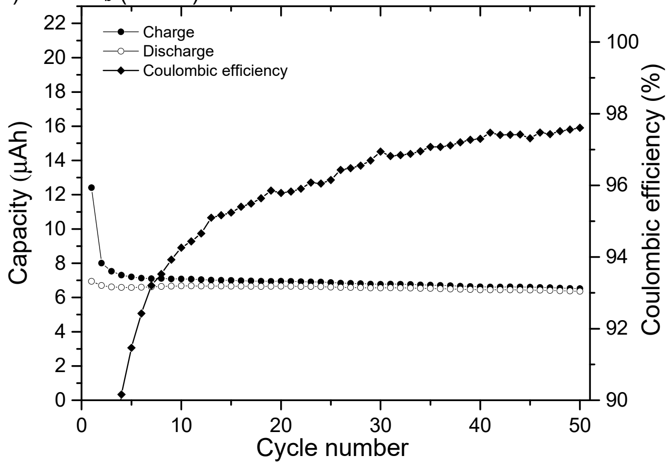
b) Coin cell/Cu_b (25165)



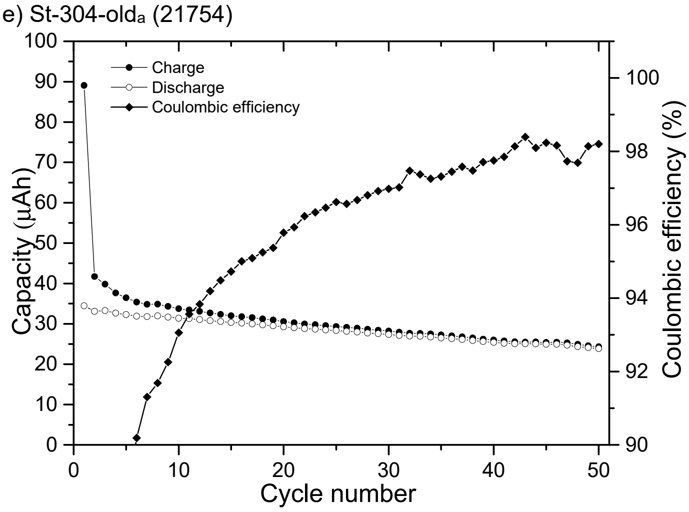
c) $Coincell_a$ (25166)



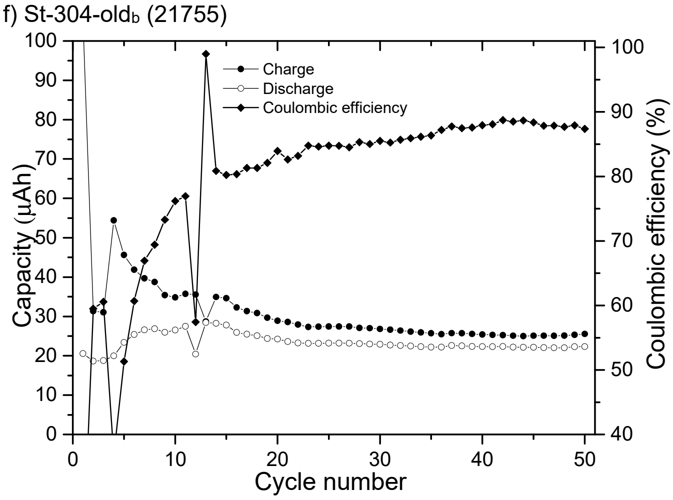
d) $coincell_b$ (25167)



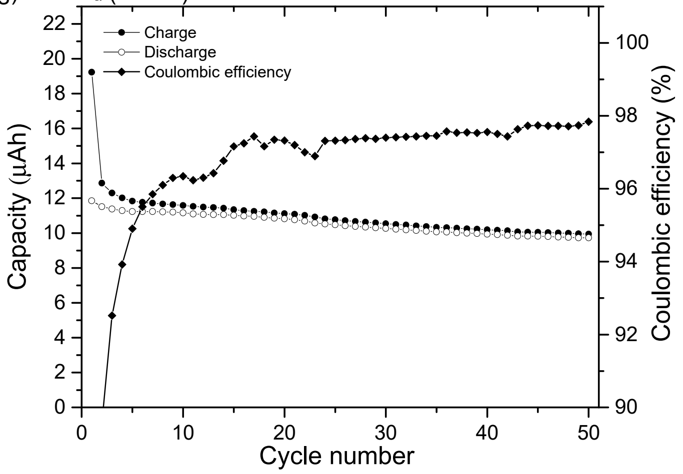
e) St-304-old_a (21754)



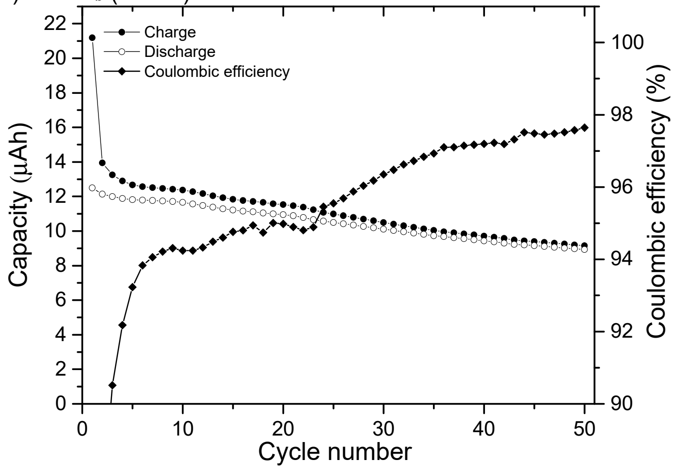
f) St-304-old_b (21755)



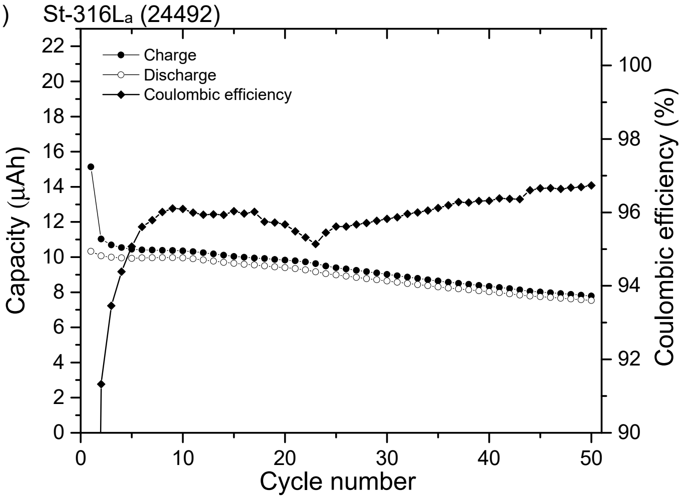
g) St-304$_a$ (24490)



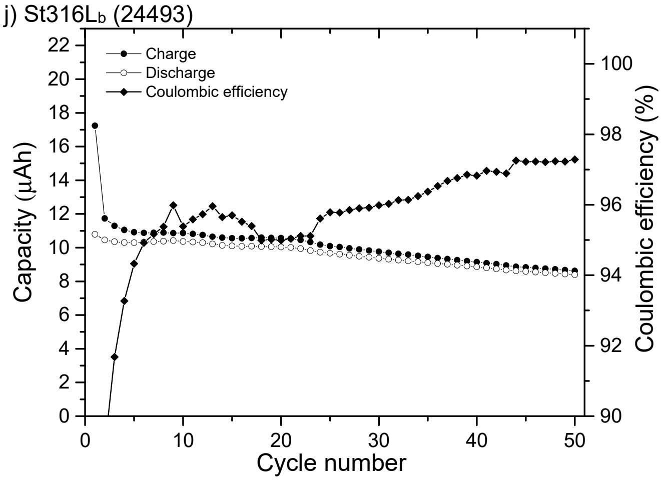
h) St-304$_b$ (24491)



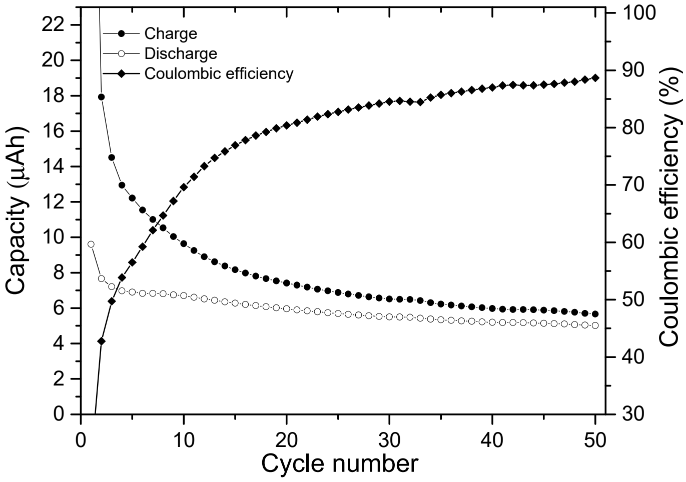
i) St-316L$_a$ (24492)



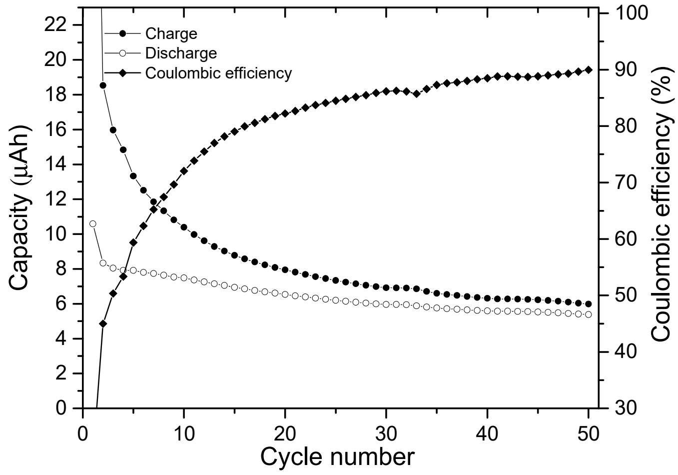
j) St316L$_b$ (24493)



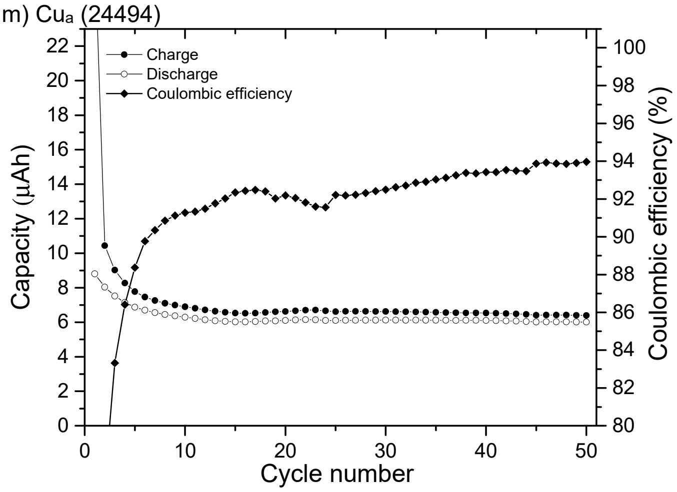
k) FeNi$_a$ (22792)



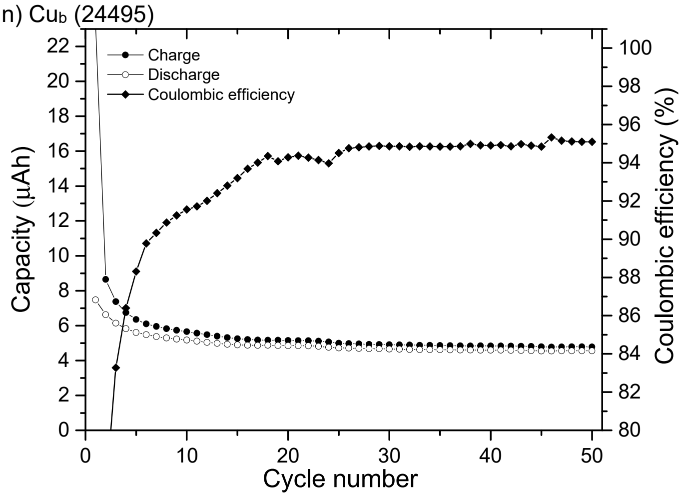
l) FeNi$_b$ (22793)



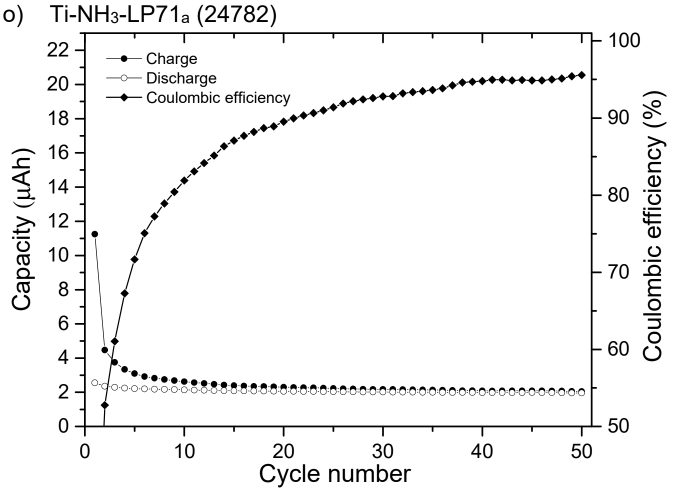
m) Cu_a (24494)



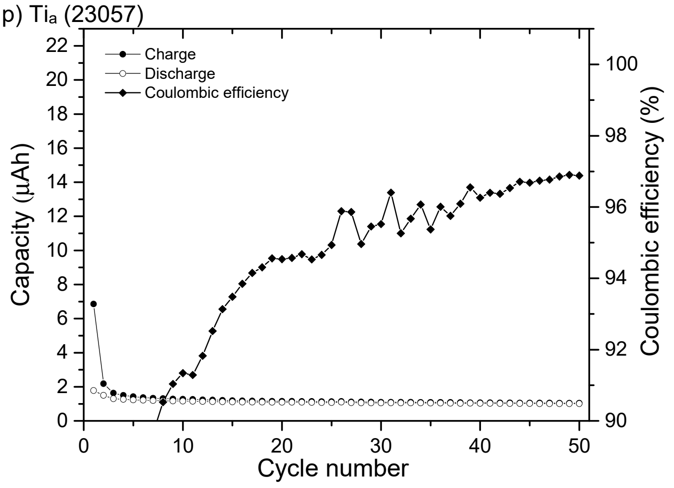
n) Cu_b (24495)



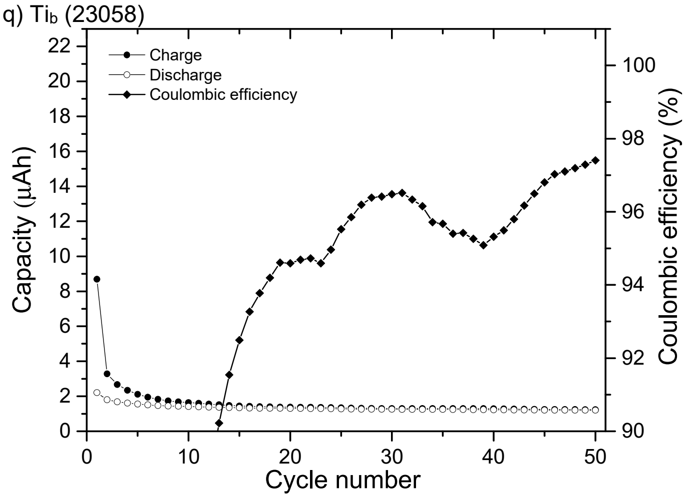
o) Ti-NH_3-$LP71_a$ (24782)



p) Ti_a (23057)



q) Ti_b (23058)



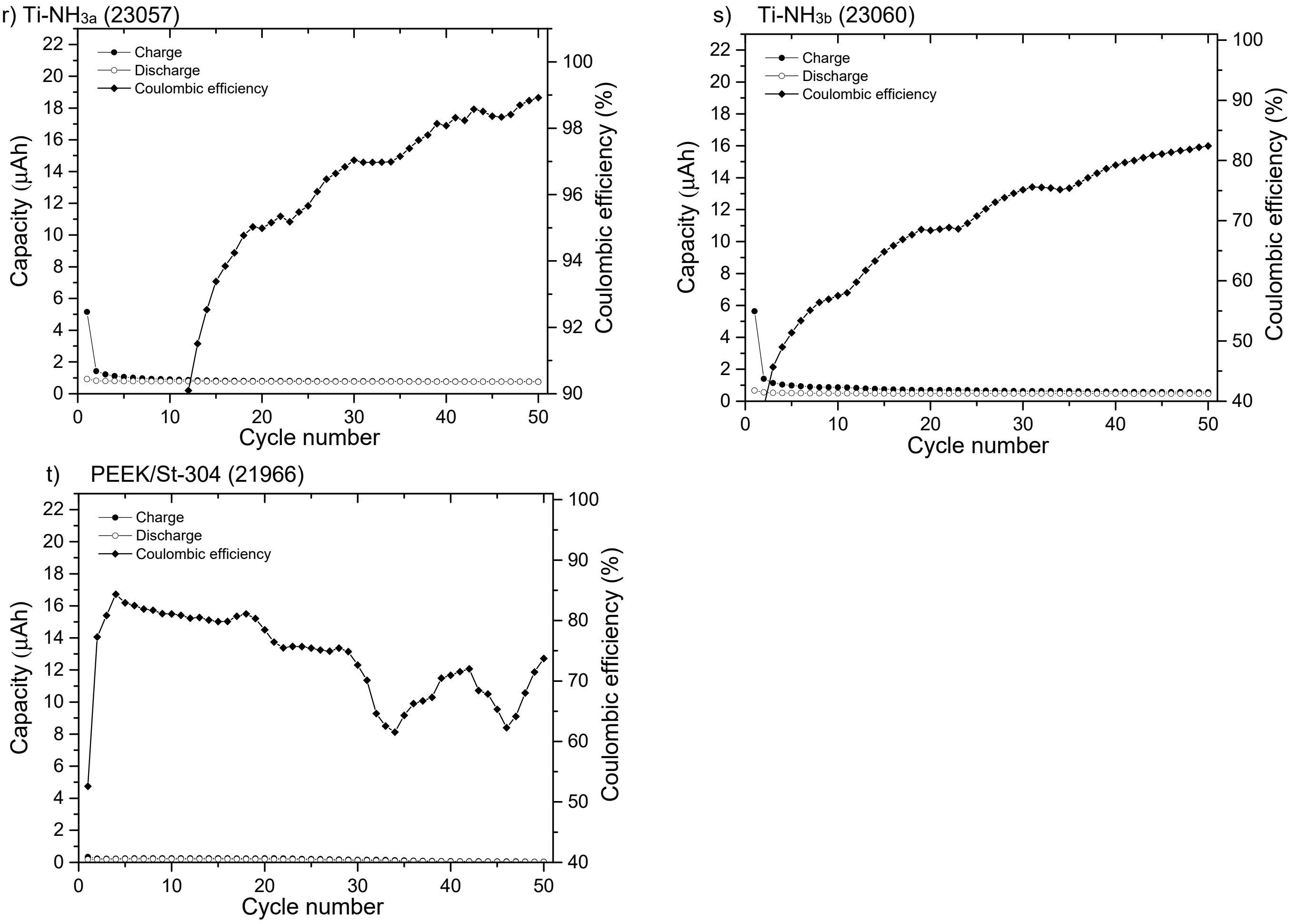
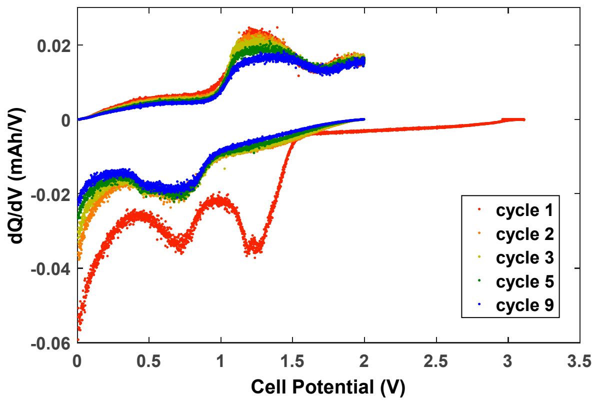


Figure S1. Detailed traces of the electrochemical cycling of the cells given in Table S2 with their charge, discharge capacity, and Coulombic efficiency. The cell reference number is given in brackets and relates to the uploaded raw data files.

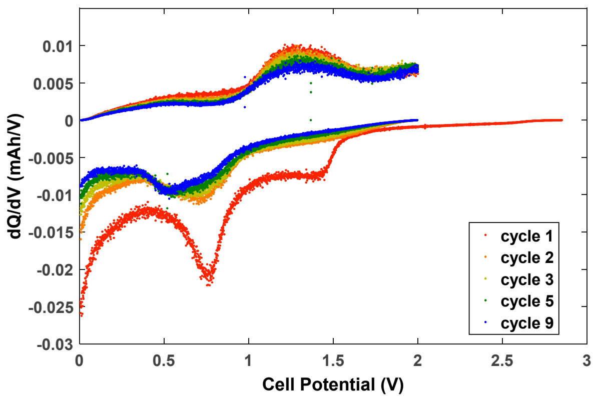
Table S4. Detailed list of electrochemical cells used to evaluate the differential capacity of the selected materials. Swagelok cell composition: Li foil, LP40 electrolyte, cycling between 5 mV to 2 V vs. Li/Li$^+$ at a constant current of 92 µA cm^{-2} for 10 cycles.

Cell number	Electrode terminal	Electrolyte	Raw data reference[3]
1	St-304_old	LP40	24496
2	St-304	LP40	24497
3	St-316	LP40	24498
4	Cu	LP40	24499
5	PEEK/St-304	LP40	24500
6	Ti	LP40	24527
7	FeNi	LP40	24528
8	TiN	LP40	23199

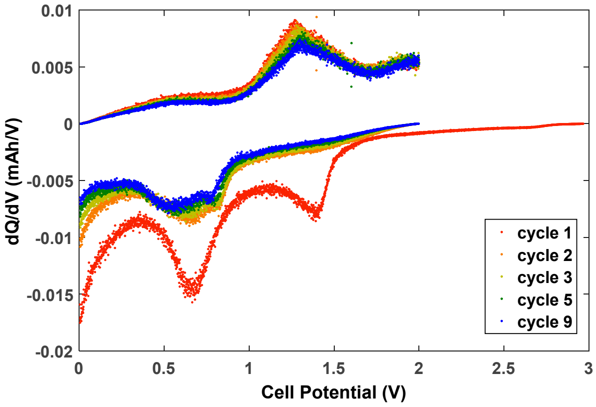
a) **St304-old (24496)**



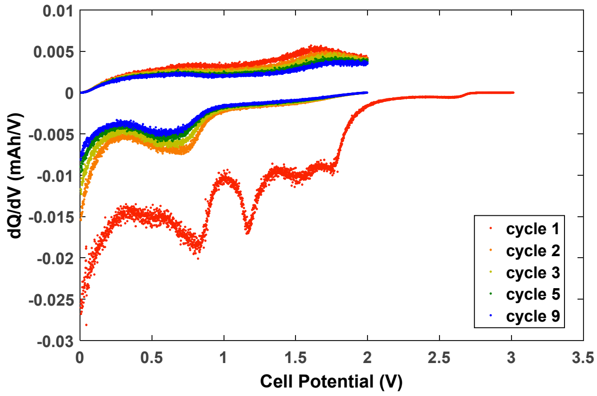
b) **St-304 (24497)**



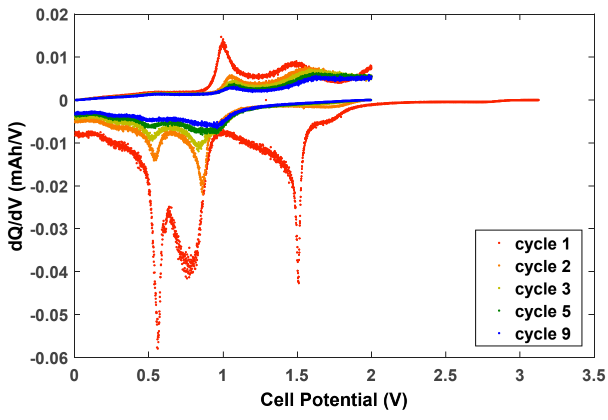
c) **St-316 (24498)**



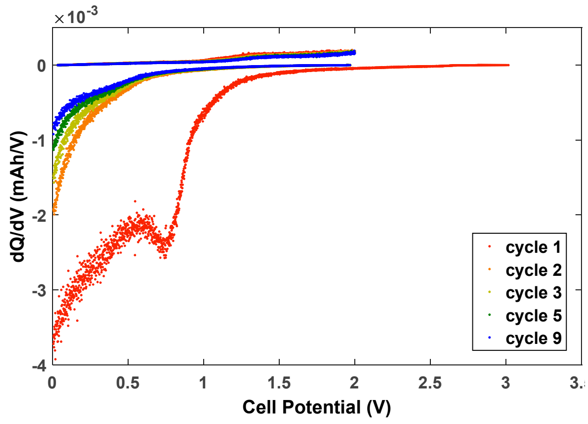
d) **Cu (24499)**



e) **FeNi (24528)**



f) **PEEK/St-304 (24500)**



g) **Ti (24527)**

h) **TiN (23199)**

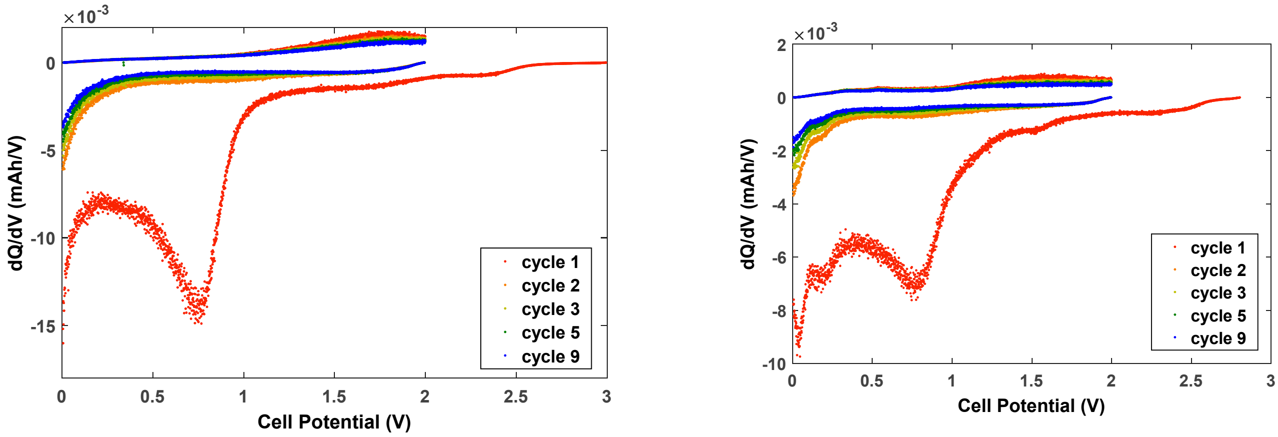


Figure S2. Detailed traces of the differential capacity plots of the cells given in Table S4.