energies

Exploring different binders for a $LiFePO_4$ battery, battery testing, modeling and simulations

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Adhesion Tests Of Lfp Coatings With Different Binders

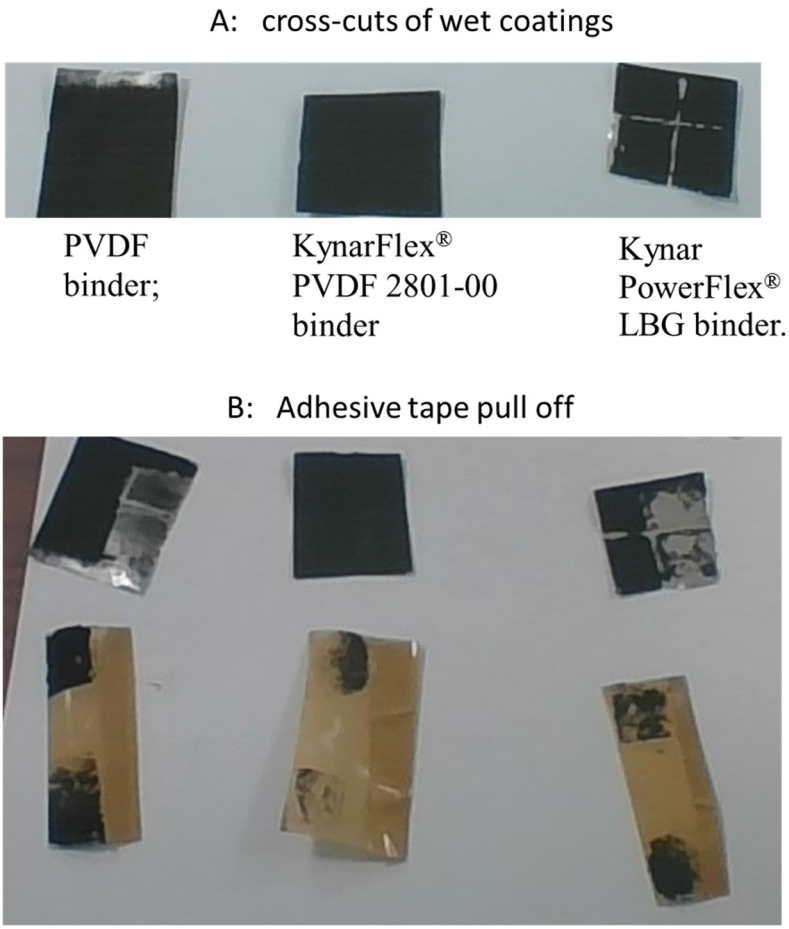

Figure S1. Results of wet adhesion test of some of the samples of LFP coatings with different types f binders: PVDF binder; B: KynarFlex® PVDF 2801-00 binder; C: Kynar PowerFlex® LBG binder.

SEM:

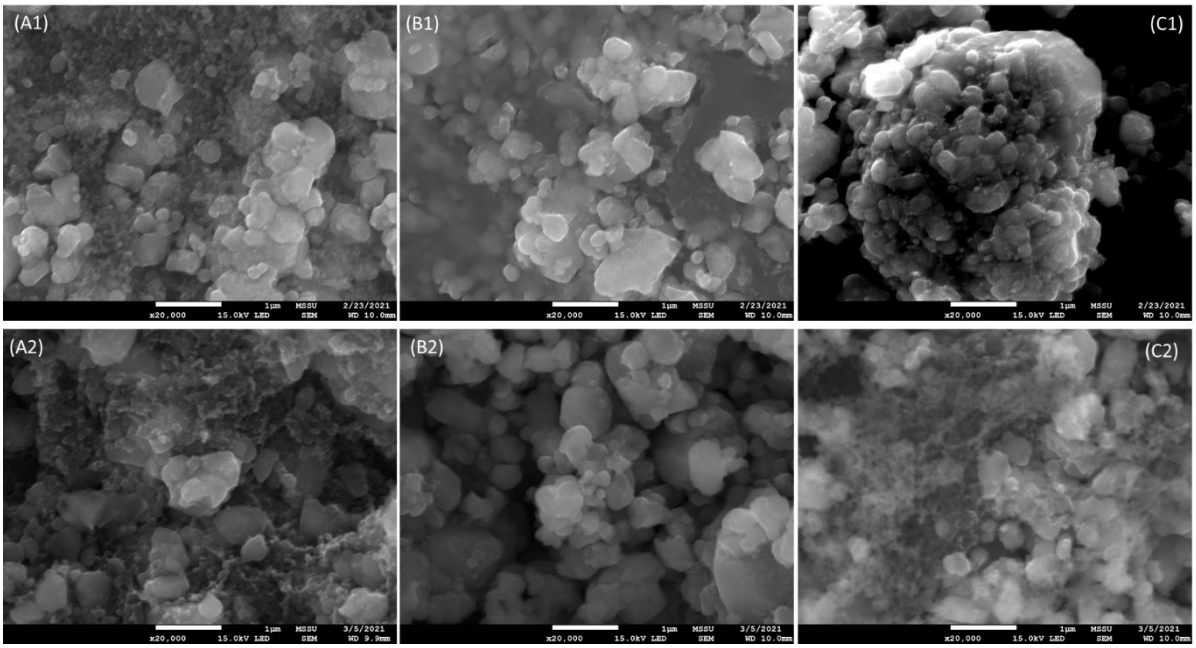

Figure S2. High magnification SEM micrographs of LFP coatings as prepared (second index: 1) and postmortem after 25 battery cell cycles (second index: 2). First index: A: PVDF binder; B: KynarFlex® PVDF 2801-00 binder; C: Kynar PowerFlex® LBG binder.

XPS Binders:

Quantification Data

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	286.4	1.45	327698.91	49.7	Y
	F1s	688.1	1.82	999759.55	50.1	Y
	O1s	532.7	3.45	3272.00	0.2	Y

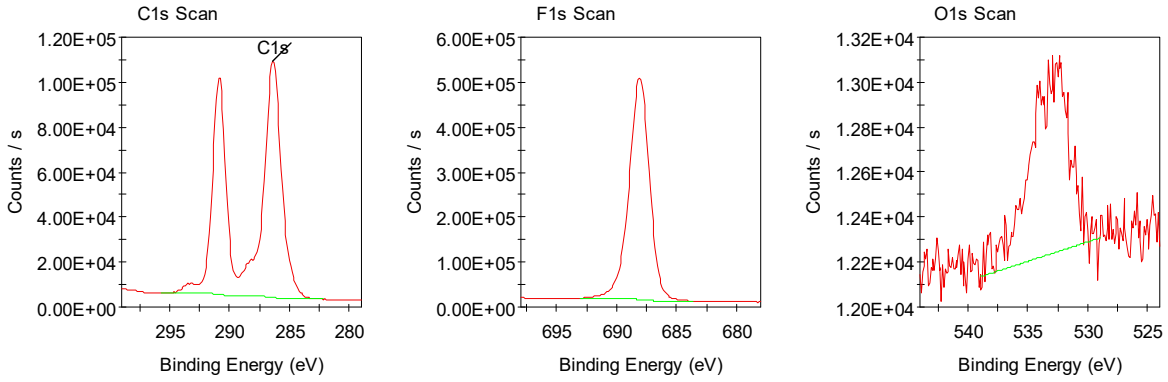

Figure S3. XPS data for the PVDF binder.

Quantification Data

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	286.4	1.49	238973.10	47.7	Y
	F1s	688.2	1.98	789223.72	52.0	Y
	O1s	533.8	2.59	3869.05	0.3	Y

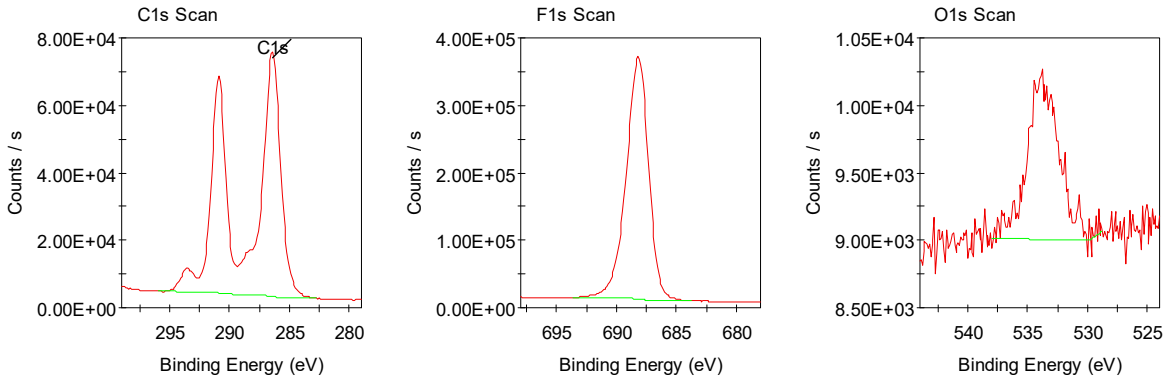

Figure S4. XPS data for the KynarFlex® PVDF 2801-00 binder.

Quantification Data

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	285.0	1.18	236061.46	53.2	Y
	F1s	688.5	2.05	179915.62	13.4	Y
	Fe3p	55.8	3.75	24489.79	3.2	Y
	N1s	400.6	1.74	1884.35	0.3	Y
	O1s	532.1	1.53	252623.61	23.6	Y
	P2p	134.1	1.79	41284.83	6.3	Y

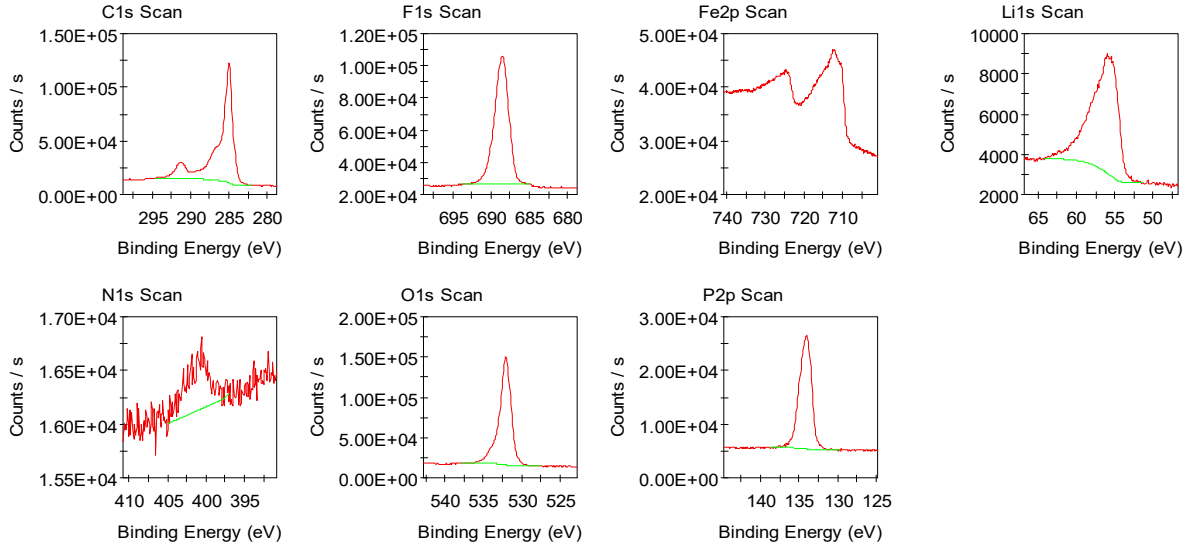

Figure S5. XPS data for the Kynar PowerFlex® LBG binder.

Table S1. XPS quantification data for coating of LFP with PVDF binder.

(a1) Coating as prepared

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	285.0	1.06	312975.77	61.9	Y
	F1s	688.2	1.81	313087.31	20.5	Y
	Fe3p	55.9	4.01	14033.24	1.6	Y
	N1s	400.9	1.70	3591.58	0.5	Y
	O1s	532.1	1.55	150184.32	12.3	Y
	P2p	134.1	1.72	23716.13	3.2	Y

(a2) Coating after 25 cycles - postmortem

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	285.0	1.59	203686.46	35.2	Y
	Cl2p	198.7	1.31	2081.49	0.1	Y
	F1s	687.9	1.91	65273.33	3.7	Y
	Li1s	55.4	1.64	10799.67	26.7	Y
	N1s	400.3	1.53	2783.01	0.3	Y
	O1s	532.0	1.64	461722.85	33.0	Y
	P2p	133.6	1.98	7597.50	0.9	Y

Table S2. XPS quantification data for coating of LFP with KynarFlex® PVDF 2801-00 binder.

(b1) Coating as prepared

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	285.3	1.98	200134.34	44.8	Y
	F1s	688.8	2.06	402245.90	29.8	Y
	Fe3p	55.7	3.54	18035.70	2.4	Y
	N1s	400.7	1.72	1290.24	0.2	Y
	O1s	532.0	1.53	194608.63	18.0	Y
	P2p	134.0	1.76	32238.24	4.9	Y

(b2) Coating after 25 cycles - postmortem

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	285.0	1.48	174683.82	32.7	Y
	Cl2p	198.8	1.45	3492.51	0.2	Y
	F1s	687.7	1.97	78170.97	4.8	Y
	Li1s	55.4	1.67	10823.98	29.0	Y
	N1s	400.1	1.29	1556.00	0.2	Y
	O1s	532.0	1.67	418805.38	32.4	Y
	P2p	133.7	1.95	5205.86	0.7	Y

Table S3. XPS quantification data for coating of LFP with Kynar PowerFlex® LBG binder.

(c1) Coating as prepared

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	285.0	1.18	236061.46	53.2	Y
	F1s	688.5	2.05	179915.62	13.4	Y
	Fe3p	55.8	3.75	24489.79	3.2	Y
	N1s	400.6	1.74	1884.35	0.3	Y
	O1s	532.1	1.53	252623.61	23.6	Y
	P2p	134.1	1.79	41284.83	6.3	Y

(c2) Coating after 25 cycles - postmortem

	Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q
	C1s	285.0	1.47	197332.68	31.1	Y
	Cl2p	198.7	1.72	7735.25	0.4	Y
	F1s	687.3	2.23	50981.44	2.7	Y
	Li1s	55.4	1.63	12999.76	29.3	Y
	N1s	399.9	2.99	3136.59	0.3	Y
	O1s	531.9	1.67	546554.54	35.6	Y
	P2p	133.8	2.22	6374.25	0.7	Y

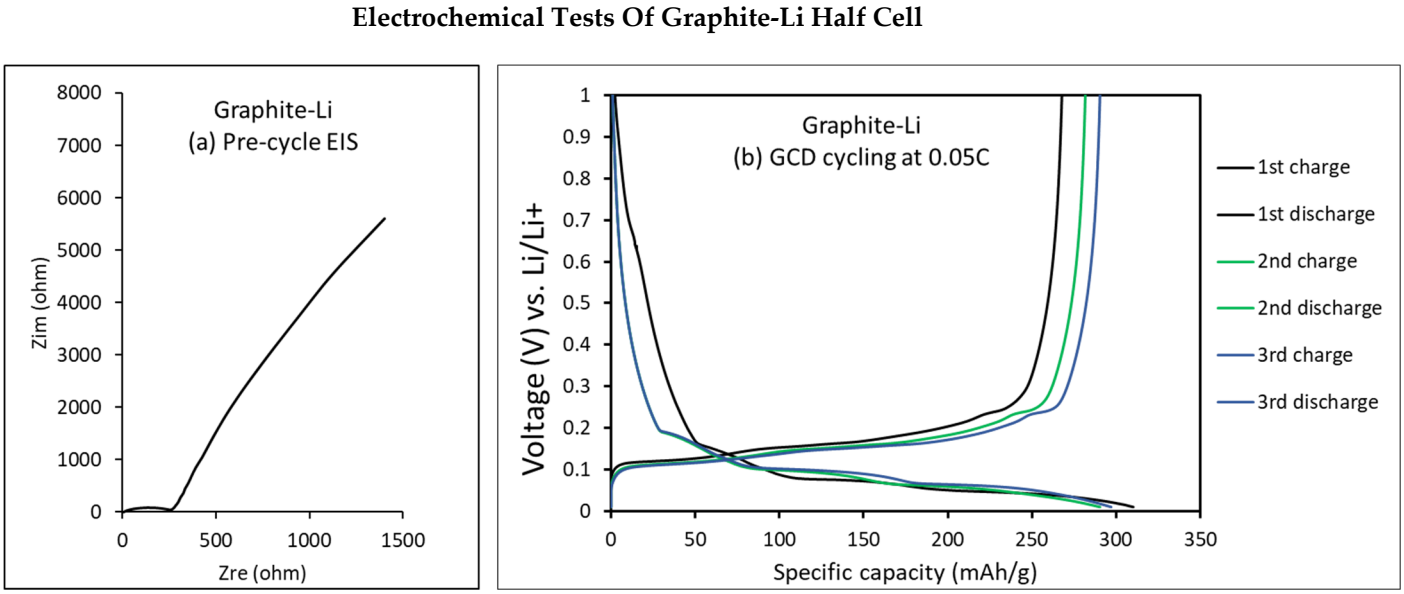

Figure S6. Nyquist plot from the EIS test and results of the GCD tests of graphite-Li half cells.

Table S4. Oxidation (charge) and reduction (discharge) plateau voltages from the GCD cycles of graphite -Li half cells.

Oxidation (o) or Reduction (r) plateau voltages	**1st Charge**	**1st Discharge**	**2nd Charge**	**2nd Discharge**	**3rd Charge**	**3rd Discharge**
P_{o1}, P_{r1} (V)	0.24	0.14	0.23	0.17	0.24	0.17
P_{o2}, P_{r2} (V)	0.16	0.087	0.15	0.1	0.15	0.1
P_{o3}, P_{r3} (V)	0.11	0.05	0.11	0.06	0.11	0.055

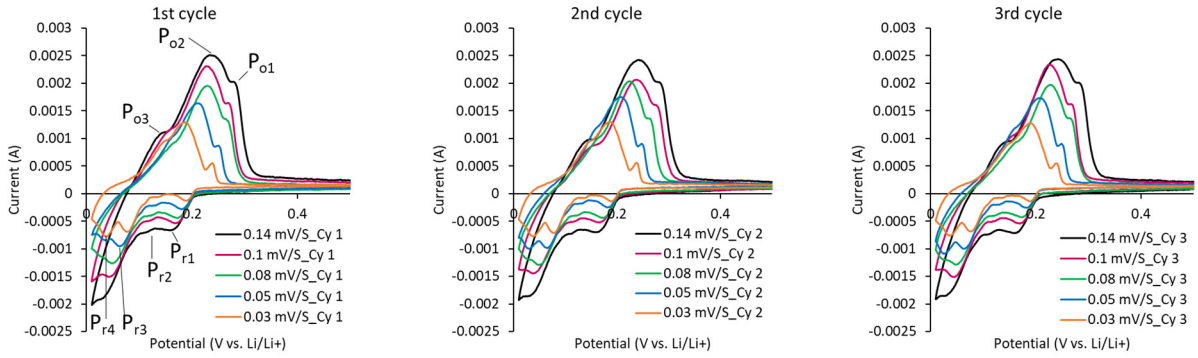

Figure S7. CV plots at different scan rates (3 cycles) of graphite-Li half cells, with the three oxidation peaks during charge and the 4 reduction peaks during discharge annotated on the first plot.

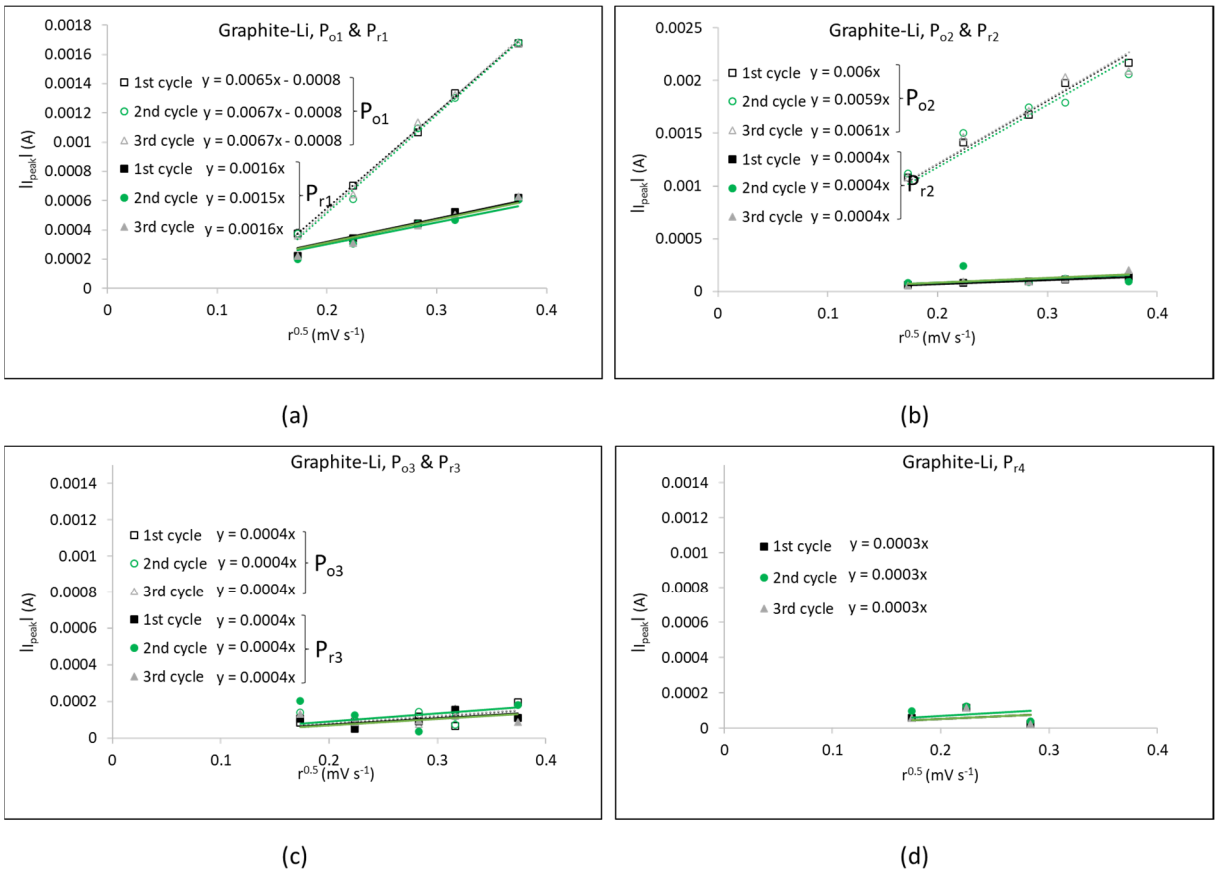

Figure S8. The linear fits of the Rendles-Shevchik equation for determining the Li^+ ion diffusion coefficient in the graphite anode for the three oxidation peaks and the four reduction peaks of the CV plots in Figure S6.

Table S5. Diffusion coefficient of the Li^+ ions in the graphite anode, determined using the Rendles-Shevchik equation and the gradient of the linear fits in Figure S7 (average of 3 cycles).

	P_{o1}	P_{r1}	P_{o2}	P_{r2}	P_{o3}	P_{r3}	P_{r4}
Diffusion coefficient (cm^2 s^{-1})	3.29×10^{-11}	1.83×10^{-12}	2.69×10^{-11}	1.20×10^{-11}	1.20×10^{-11}	1.20×10^{-11}	6.73×10^{-12}

Equivalent Electric Circuit Model (Eecm)

Table S6. Fitted parameters of the EECM against experimental EIS data, pre-cycling and after 5 GCD cycles of a graphite-LFP cell.

EECM Parameter		Pre-cycling	After 5 GCD cycles
R1 (ohm)		200	10
R2 (ohm)		73	73
CPE1: Q1 (S s^{n1}),	n1	43.8×10^{-6}, 0.765	17×10^{-6}, 0.825
R3 (ohm)		367	184
CPE2: Q2 (S s^{n2}),	n2	291×10^{-6}, 0.8	66×10^{-6}, 0.845
R4 (ohm)		52	97
CPE3: Q3 (S s^{n3}),	n3	680×10^{-6}, 0.757	89×10^{-6}, 1
CPE4: Q4 (S s^{n4}),	n4	724×10^{-6}, 0.983	932×10^{-6}, 0.260
R5 (ohm)			11570
CPE5: Q5 (S s^{n5}),	n5		583×10^{-3}, 0.995
CPE6: Q6 (S s^{n6}),	n6		32×10^{-6}, 0.726
CPE7: Q7 (S s^{n7}),	n7	113×10^{-3}, 0.300	113×10^{-3}, 0.300

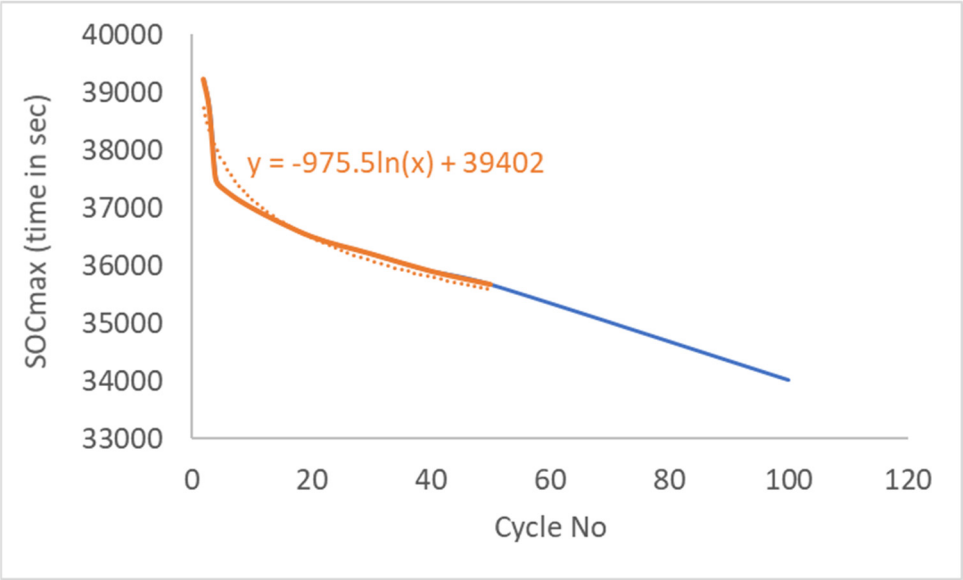

Figure S9. Experimental data of maximum SOC of graphite-LFP battery cell as a function of cycle number (orange solid line: up to 50 cycles, blue solid lines to 100 cycles) and fit of the experimental data up to 50 cycles (orange broken line with the equation displayed on the graph).