

Supporting Information

Silicon Carboxylate derived Silicon Oxycarbides as Anodes for Lithium Ion Batteries

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Table S1. Residual weights for several batches

Sample	Initial weight		Residual weight after		Residual weight after	
			heating to 250°C		carbonisation	
	STA [mg]	CA [mg]	[g]	[%]*	[g]	[%]*
SiCO_0	2545	---	563	78	327	13
SiCO_0	2538	---	831	67	474	19
SiCO_0	2487	---	574	76	369	15
SiCO_1.3	2520	813	1269	62	743	29
SiCO_1.3	2509	817	1283	61	746	30
SiCO_1.3	2505	810	1312	60	---	---
SiCO_1.3	1240	438	631	61	---	---
SiCO_2.5	2501	1499	1610	60	793	32
SiCO_2.5	2513	1515	1463	63	805	32
SiCO_2.5	993	611	523	67	306	31
SiCO_4	2516	2420	1439	71	689	27
SiCO_4	2504	2418	1128	77	682	27
SiCO_4	1095	1143	510	62	313	29

*The percentual residual weights are related to the sum of STA+CA.

Table S2. Active material loadings for all electrochemical measurements

Figure	Sample	Binder	SLMP® content [mg/g _{Active material}]	Electrode composition Active material/binder/carbon black [wt%/wt%/wt%]	Active material loading [mgcm ⁻²]
4a	SiCO_0	PVDF		80/10/10	1.41
	SiCO_1.3	PVDF		80/10/10	1.72
4b	SiCO_1.3	PVDF		80/10/10	1.95
4c	SiCO_1.3	PVDF		80/10/10	1.72
	SiCO_0	PVDF		80/10/10	1.41
	Graphite	PVDF		80/10/10	1.80
4d	SiCO_1.3	PVDF		80/10/10	1.72
	SiCO_2.5	PVDF		80/10/10	2.99
	SiCO_4	PVDF		80/10/10	1.70
5a	SiCO_1.3	LiPAA		75/15/10	1.64
5b	SiCO_1.3	LiPAA		75/15/10	1.69
5c	SiCO_1.3	LiPAA		75/15/10	1.64
	SiCO_1.3	LiPAA	189	75/15/10	1.73
	SiCO_1.3	LiPAA	348	75/15/10	1.72
	SiCO_1.3	LiPAA	382	75/15/10	1.70
S2	SiCO_1.3	PVDF		80/10/10	1.72
	SiCO_1.3	LiPAA		75/15/10	1.92

Table S3. NMR data for distillates

Sample	Chemical shifts [ppm]		
	¹ H-NMR	¹³ C-NMR	²⁹ Si-NMR
Silicon tetraacetate	2.16 (CH ₃)	22.24 (CH ₃), 167.81 (COOH)	96.36
Acetic acid (AA)	2.10 (CH ₃)	20.81 (CH ₃), 175.99 (COOH)	n.d.
Acetic anhydride (AN)	2.23 (CH ₃)	22.15 (CH ₃), 166.38 (COOH)	n.d.
SiCO_0	2.06 (CH ₃ -AA), 2.19 (CH ₃ - AN)	20.62 (CH ₃ -AA), 22.11 (CH ₃ -AN), 166.4 (COOH-AN)	n.d.
SiCO_1.3	2.09 (CH ₃ -AA), 2.21 (CH ₃ - AN)	20.83 (CH ₃ -AA), 22.16 (CH ₃ -AN), 166.47 (COOH-AN), 177.88 (COOH-AA)	n.d.

Table. S4. XPS data for unsputtered SiCO samples

Sample	Carbon content from XPS analysis [wt%]	Molar O/Si ratio
SiCO_0	13.96	1.99
SiCO_1.3	29.96	2.13
SiCO_2.5	30.07	2.19
SiCO_4	23.60	2.00

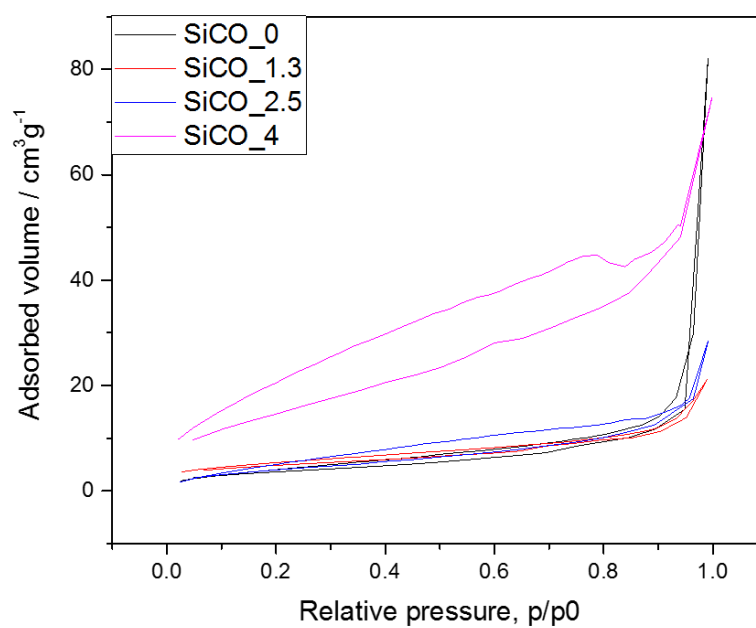


Fig. S1. Sorption isotherms for the SiCO samples.

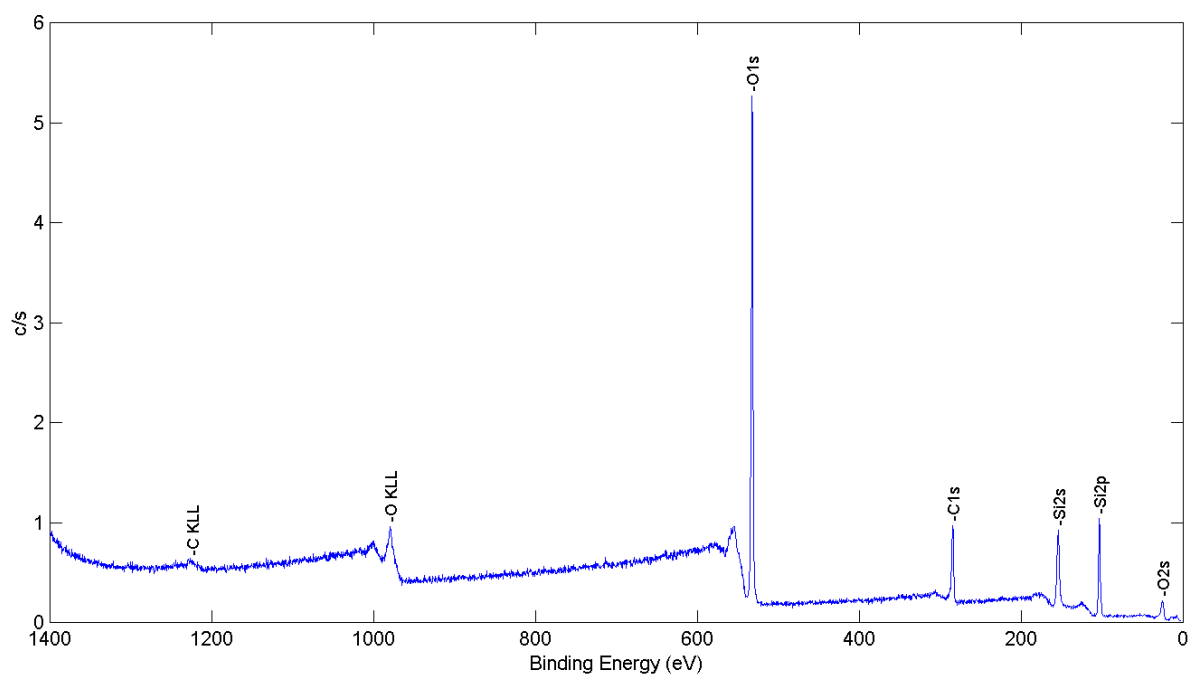


Fig. S2a. XPS survey spectrum for non-sputtered SiCO₀

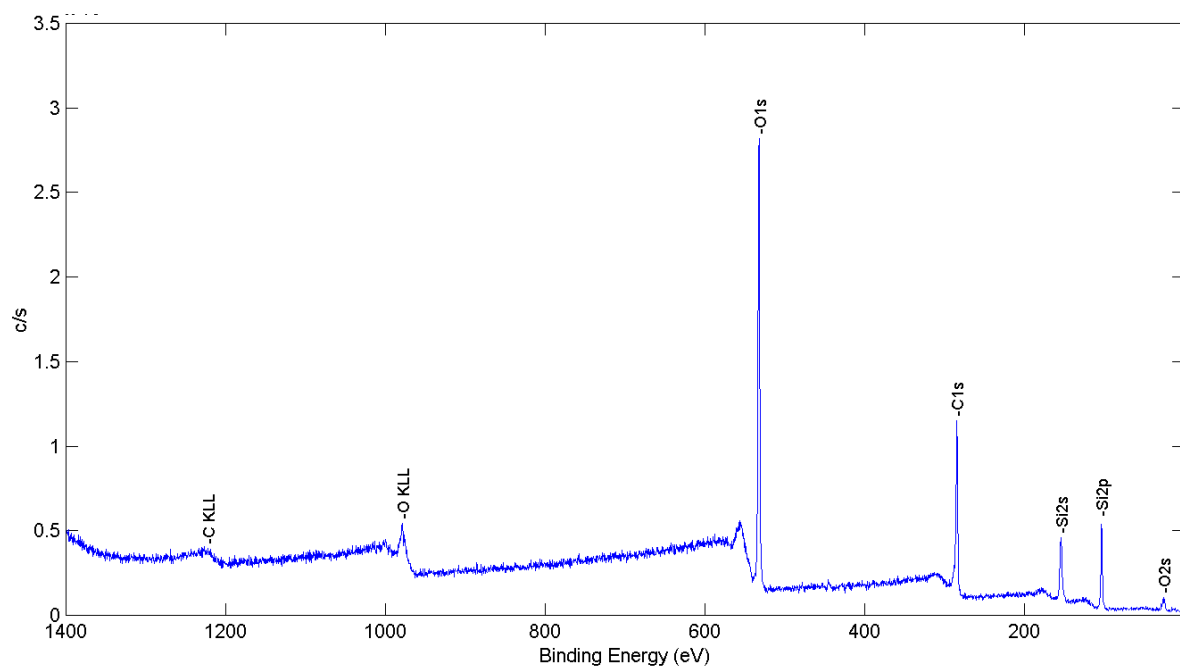


Fig. S2b. XPS survey spectrum for non-sputtered SiCO_{1.3}

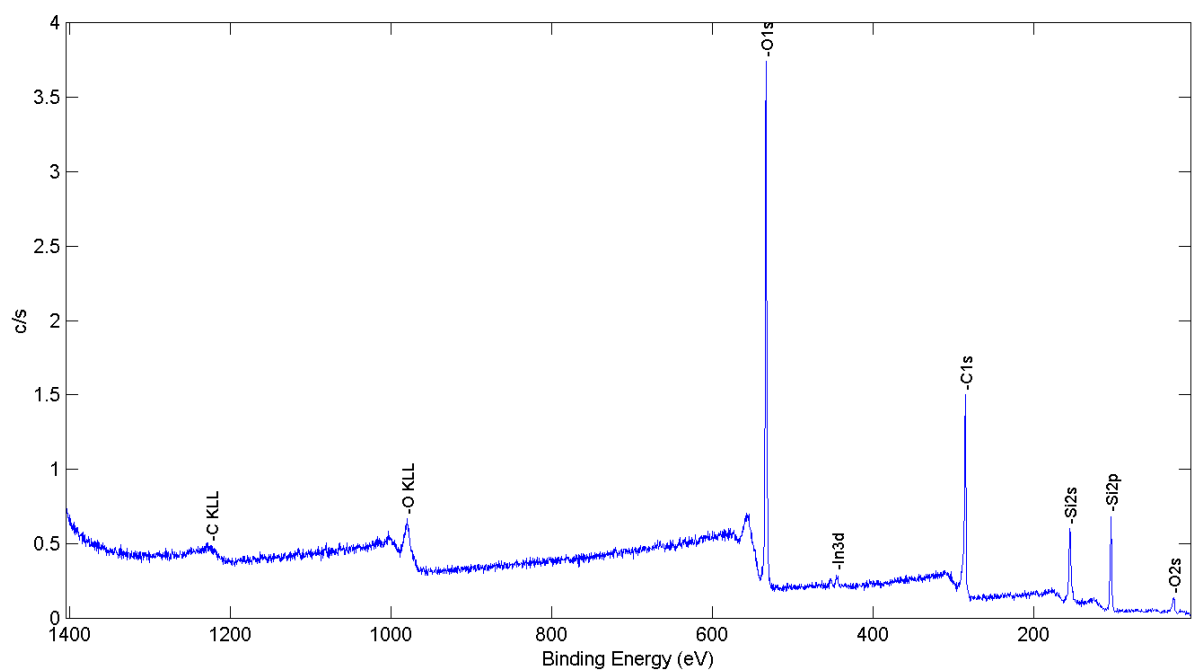


Fig. S2c. XPS survey spectrum for non-sputtered SiCO_{2.5}

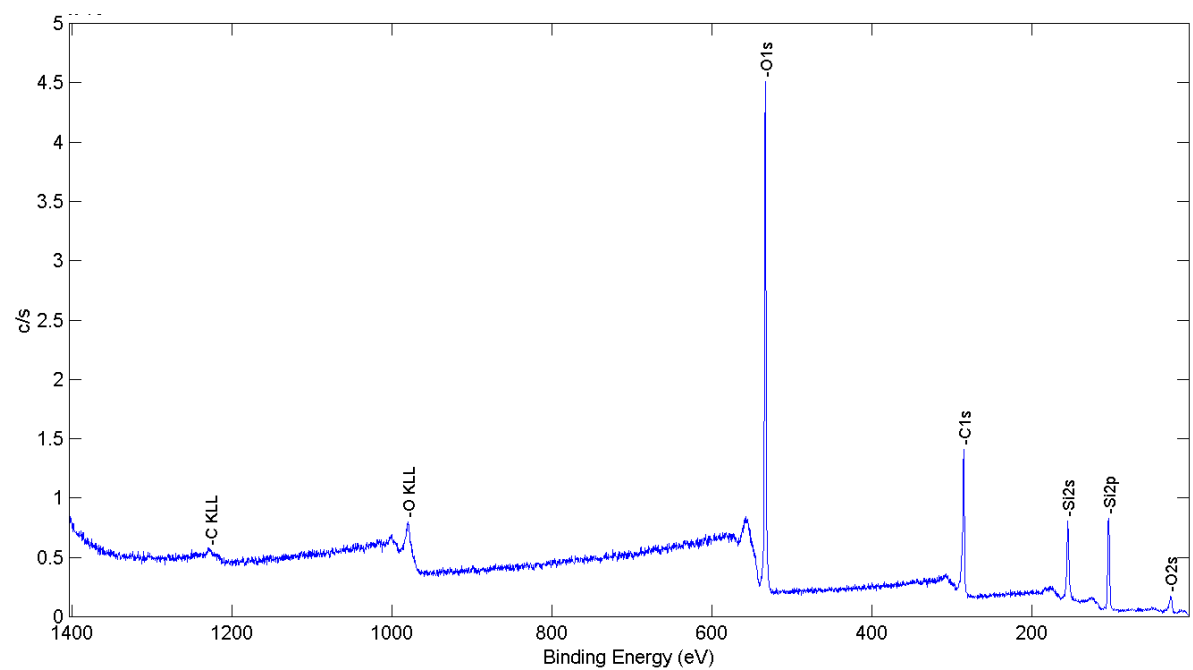


Fig. S2d. XPS survey spectrum for non-sputtered SiCO₄

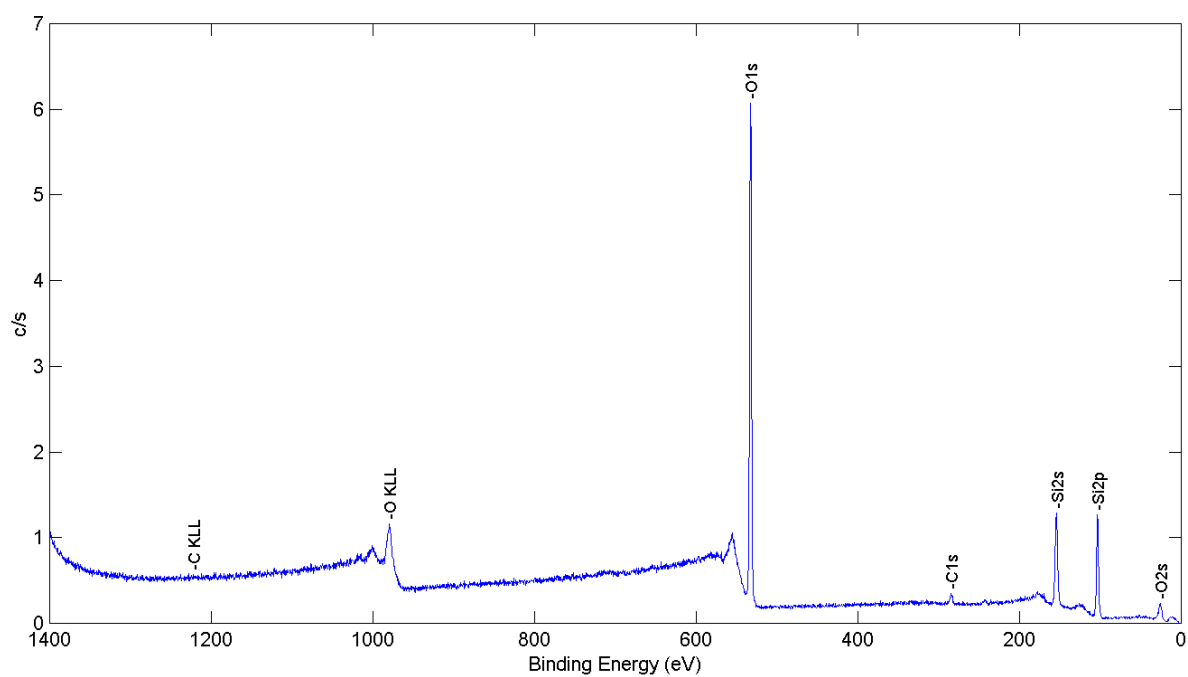


Fig. S2e. XPS survey spectrum for sputtered SiCO₀

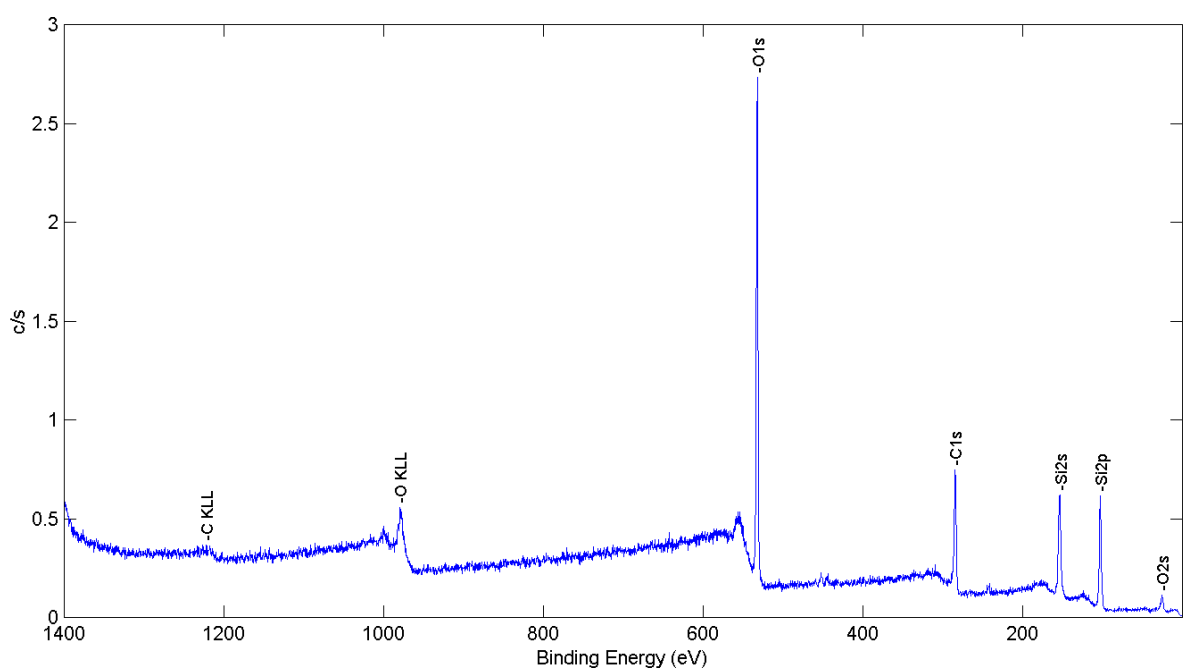


Fig. S2f. XPS survey spectrum for sputtered SiCO_{1.3}

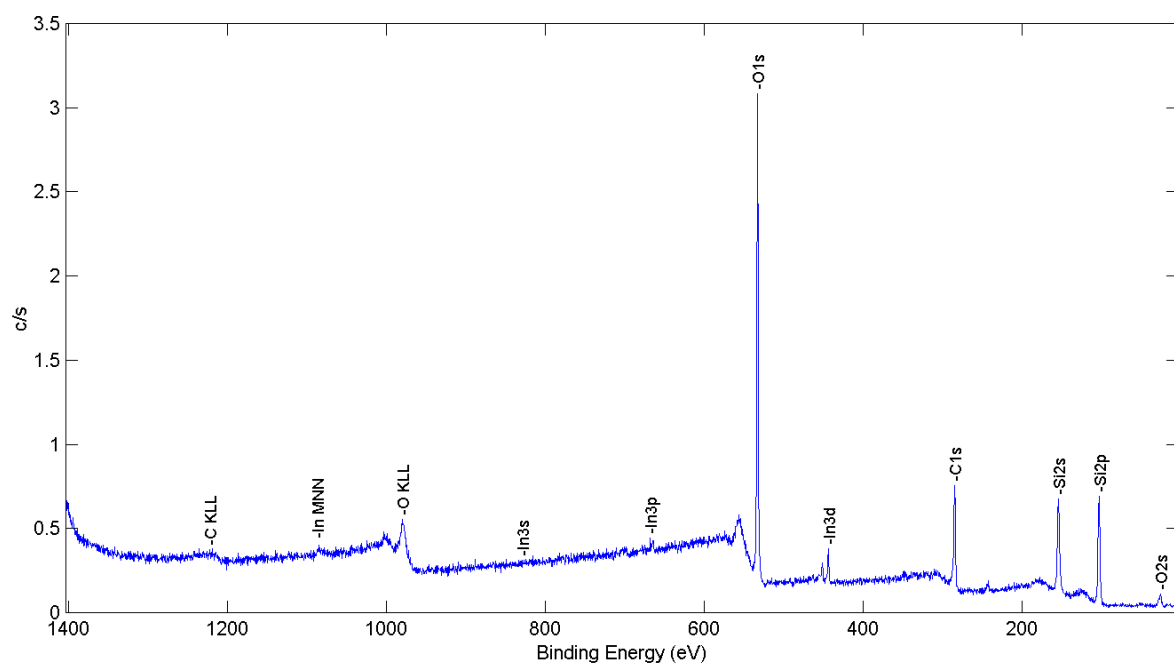


Fig. S2g. XPS survey spectrum for sputtered SiCO_{2.5}

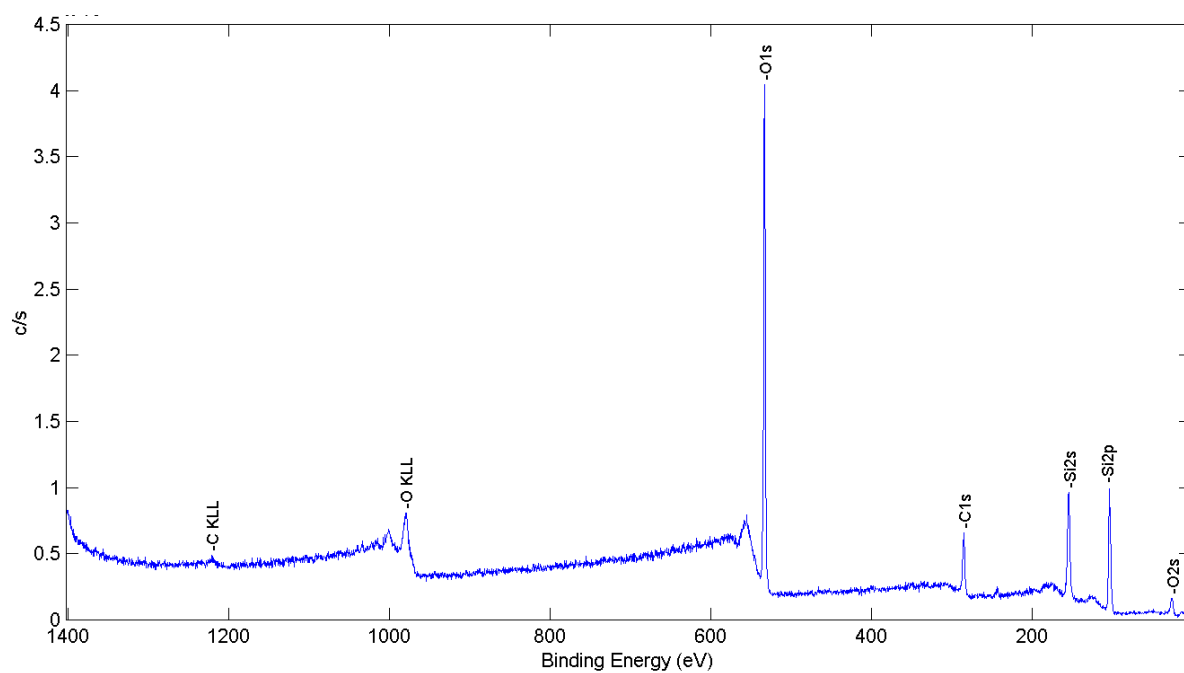


Fig. S2h. XPS survey spectrum for sputtered SiCO₄

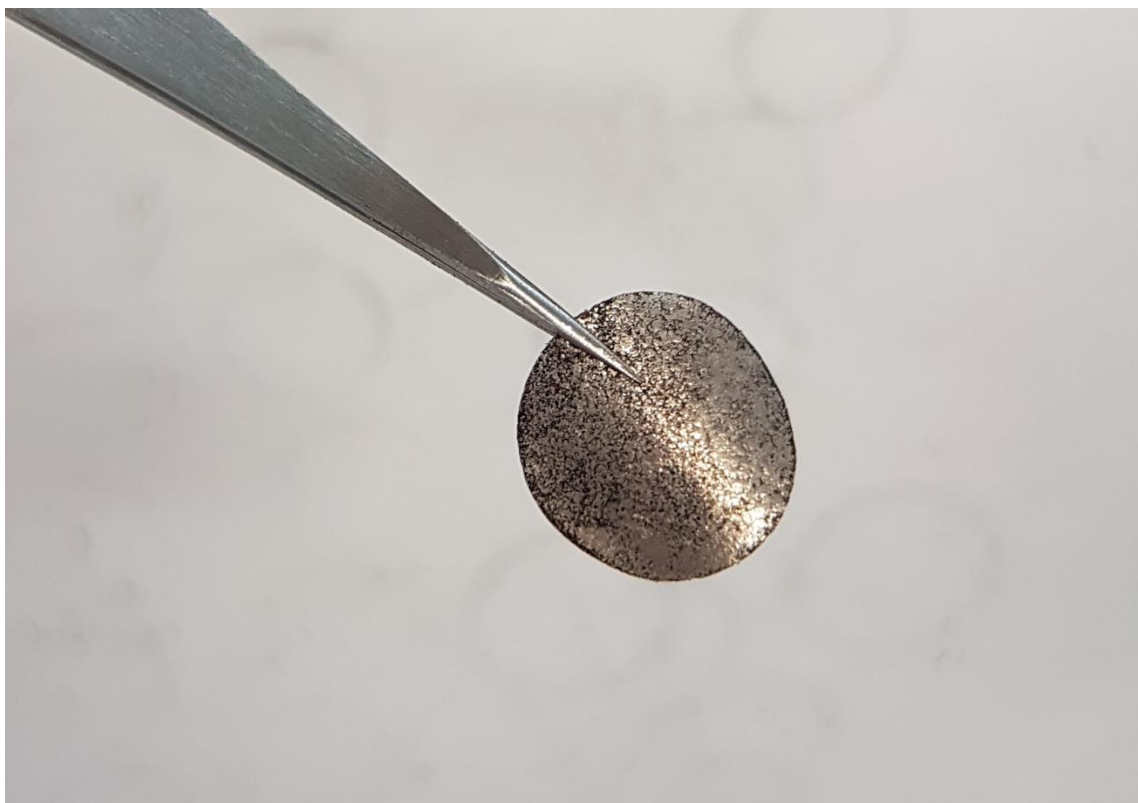


Fig. S3. Photograph of a prelithiated electrode. SLMP[®] loading: 366 mg/g_{Active material}.

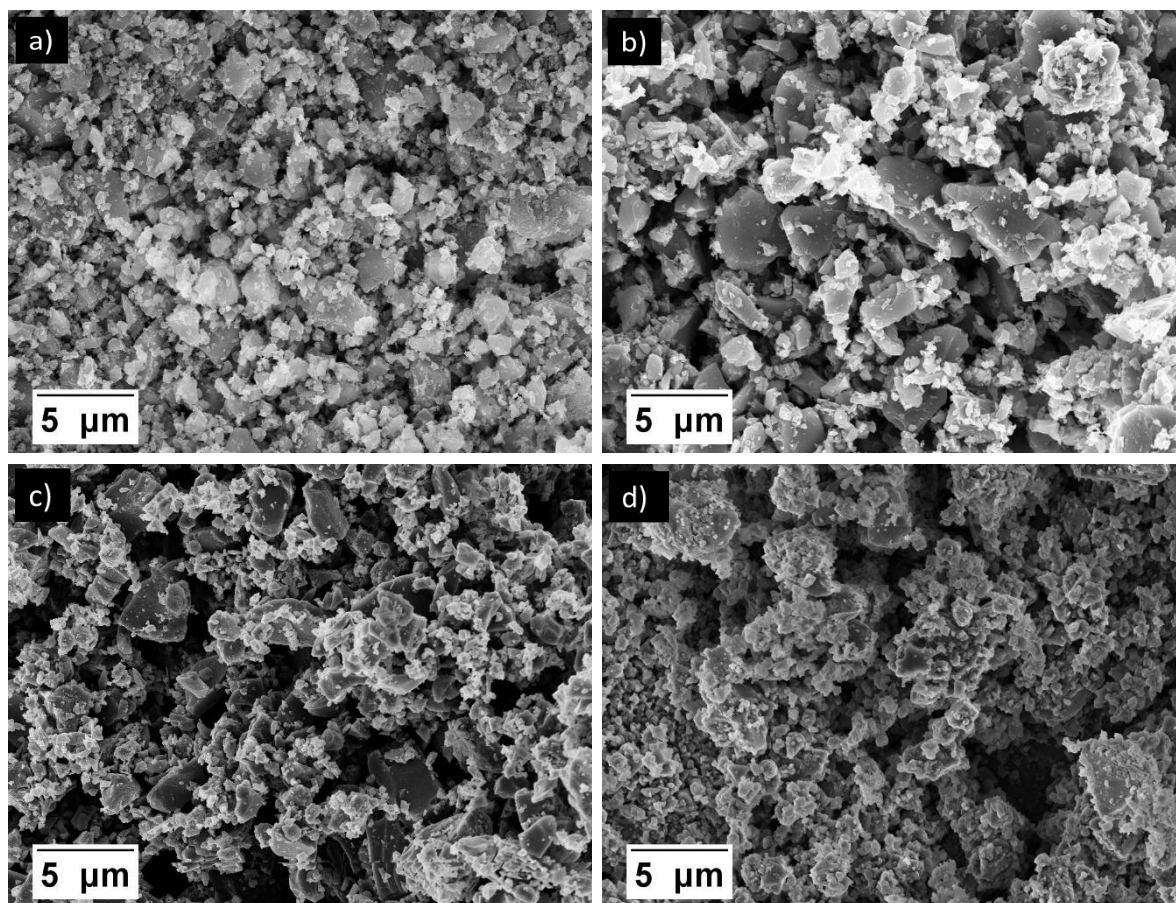


Fig. S4. SEM images of SiCO samples. a) SiCO_0, b) SiCO_1.3, c) SiCO_2.5 and d) SiCO_4.

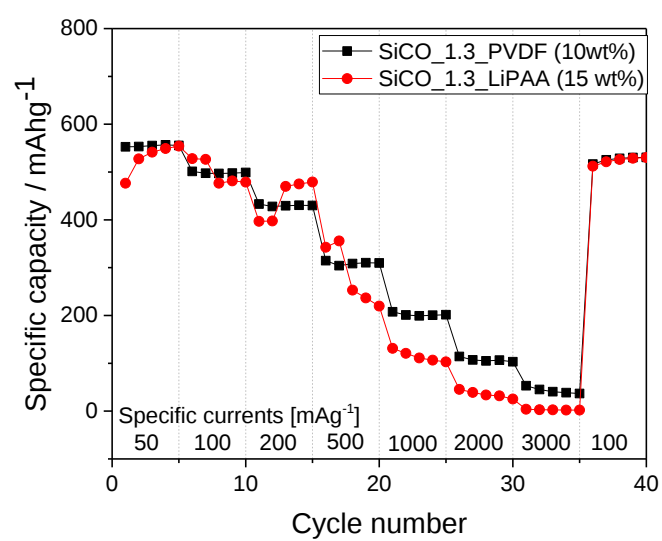


Fig. S5. Comparison of rate capability for SiCO_{1.3} electrodes prepared with PVDF and LiPAA binder.