A Si@SiOC@Li₂Si₂O₅ Anode Derived from Pyrolysis of Polysiloxane Enables Lithium-ion Batteries with High Electrochemical Performance and High Initial Coulombic Efficiency

Longsheng Li, Yue Zhang, Wen Chen, Wei Yang, Hanbo Zou, Tianxing Kang*, Shengzhou Chen*

College of Chemistry and Chemical Engineering, Guangzhou University, Guangzhou 510006, Guangdong, China;

*Corresponding author,

E-mail address: txkang@gzhu.edu.cn; Phone: +86-15521164893

E-mail address: szchen@gzhu.edu.cn; Phone: +86-13342884267

Address: Guangzhou University, 230 Waihuan West Road, Fanyu District, Guangzhou

510006, Guangdong Province, China



Figure S1. (a) FT-IR spectra of the SiOC and SSS. (b) XRD patterns of the SiOC and SSS. (c) Raman spectra of the SiOC and SSS.



Figure S2. Element distribution spectra of the SSL.

	First		Reversible	
Sample (current density mA g ⁻¹)	reversible capacity	ICE(%)	capacity (after N cycles)	Reference
	$(mAh g^{-1})$			
Pure SiOC				
SiOC-Ar (36)	760	50	>400 (100)	Graczyk-zajac et al. 2018 (ref. 1) ¹
SiOC-DVB-1 (100)	819	65	476 (500)	Wu et al. 2022 (ref. 2) ²
SiOC-500 (100)	578	57	351 (200)	Xia et al. 2020 (ref. 3) ³
Carbon based SiOC com	posites			
SiOC:C nanohybrids (50)	436	54	470 (50)	Wang et al. 2015 (ref. 4) ⁴
SiOC/C NF-0.5(100)	1011	68	707 (200)	Huang et al. 2021 (ref. 5)
Onion-like SiOC/C (100)	658	78	540 (50)	Lin et al. 2022 (ref. 6) ⁶
Graphite based SiOC con	nposites			
SiOC/graphite (SG)(50)	580	71	480 (1000)	Wu et al. 2019 (ref. 7) ⁷
NCG@SiOC (372)	520	72	300 (1000)	Hong et al. 2021 (ref. 8) 8
SiOCPhTES/C10g (186)	452	54	293 (20)	Knozowski et al. 2020 (re 9) ⁹
Graphene oxide/reduced	graphene oxi	ide/graphe	ne based SiOC	composites
SiOC@C/graphene(200)	674	62	691 (100)	Ma et al. 2022 (ref. 10) ¹⁰
3D GNS SiOC (100)	844	66	701 (100)	Sang et al. 2018 (ref. 11) ¹
NGA SiOC 25 (37)	747	67	605 (90)	Shao et al. 2020 (ref. 12) ¹
Si/SiOC composites				
SiOC. N–Si-a (74)	704	-	620 (100)	Kaspar et al. 2014 (ref. 13) ¹³
Sitc:SiOC (-)	593	65	289 (50)	Vrankovic et al. 2017 (ref. 14) ¹⁴
Si/SiOC-0.6 (100)	980	63	800 (100)	Wu et al. 2019 (ref. 15) ¹⁵
Sn/SiOC composites				
1.1 Sn- SiOCfiber	939	82	457 (100)	Tolosa et al. 2018 (ref. 16) ¹⁶
Sn@SiOC NPs (186)	656	67	411 (250)	Xia et al. 2020 (ref. 17) ¹⁷
SiOC:C0.2/Sn-40% (100)	439	56	351 (100)	Knozowski et al. 2022 (re 18) ¹⁸
This work				,
$Si@SiO_x(500)$	2773	87	0 (80)	
SSL (500)	983	73	733 (500)	
SiOC (500)	639	55	205 (500)	
SSS (500)	1082	70	170 (500)	

Table S1. Electrochemical performance of SiOC-based composites.



Figure S3. The CV curves for the initial three cycles of (a)SiOC, (b) SSS between 3.0 and 0.001 V (vs. Li/Li⁺) at a scan rate of 0.1 mV s⁻¹. (c) ICE the SiOC and SSS anodes. Charge/discharge voltage profiles of (d) SiOC, (e) SSS electrodes at specific current values from 0.1 to 2 A g⁻¹. (f) Rate performance of the SiOC and SSS anodes. (g) Cycling performance of SiOC and SSS electrodes at 0.5 A g⁻¹.

C		
Electrode material	Rct/Ω	Rs/Ω
Si@SiO _x -1st	28.95	3.885
SSL-1st	6.132	3.573
$Si@SiO_x$ -500th	18.02	15.35
SSL-500th	9.322	10.71
SiOC-1st	35.39	3.541
SSS-1st	15.64	3.109

Table S2. R_{ct} and R_s values for Si@SiO_x, SSL, SiOC and SSS electrodes in EIS tests.

Table S3. R_{ct} and R_s values of SSL electrodes over 500 cycles.

Number of cycles	Rct/Ω	Rs/Ω
After 1 cycle	6.132	3.573
After 10 cycles	7.52	4.759
After 20 cycles	6.597	3.72
After 50 cycles	7.336	3.618
After 100 cycles	7.71	4.007
After 200 cycles	9.001	7.238
After 500 cycles	9.322	10.71

References

- 1. M. Graczyk-Zajac, D. Vrankovic, P. Waleska, C. Hess, P. V. Sasikumar, S. Lauterbach, H.-J. Kleebe and G. D. Sorarù, *Journal of Materials Chemistry A*, 2018, **6**, 93-103.
- 2. P. Wu, X. Guo, Z. Su, C. Liu, S. Chen, Z. Zheng and A. Liu, *Chemical Engineering Journal*, 2022, 446.
- 3. Y. Xia, S. Cai, C. Lu, H. Huang, Y. Gan, J. Zhang, C. Liang, Z. Xiao and W. Zhang, *Journal of Alloys and Compounds*, 2020, **816**.
- 4. J. Wang, C. Luo, T. Gao, A. Langrock, A. C. Mignerey and C. Wang, *Small*, 2015, **11**, 473-481.
- 5. X. Huang, B. Christopher, S. Chai, X. Xie, S. Luo, S. Liang and A. Pan, *ACS Applied Energy Materials*, 2021, **4**, 1677-1686.
- 6. X. Lin, Y. Dong, X. Liu, X. Chen, A. Li and H. Song, *Chemical Engineering Journal*, 2022, **428**.
- 7. Z. Wu, X. Cheng, D. Tian, T. Gao, W. He and C. Yang, *Chemical Engineering Journal*, 2019, **375**.
- 8. H. Hong, W. Liu, M. Zhang, Y. Wang and Y. Chen, *Journal of Alloys and Compounds*, 2021, **857**.
- 9. D. Knozowski, M. Graczyk-Zajac, G. Trykowski and M. Wilamowska-Zawlocka, *Materials (Basel)*, 2020, **13**.
- 10. M. Ma, H. Wang, L. Xiong, S. Huang, X. Li and X. Du, *Carbon*, 2022, **186**, 273-281.
- 11. Z. Sang, Z. Zhao, D. Su, P. Miao, F. Zhang, H. Ji and X. Yan, *Journal of Materials Chemistry A*, 2018, **6**, 9064-9073.
- G. Shao, D. A. H. Hanaor, J. Wang, D. Kober, S. Li, X. Wang, X. Shen, M. F. Bekheet and A. Gurlo, *Acs Applied Materials & Interfaces*, 2020, 12, 46045-46056.
- 13. J. Kaspar, M. Graczyk-Zajac, S. Lauterbach, H.-J. Kleebe and R. Riedel, *Journal of Power Sources*, 2014, **269**, 164-172.
- D. Vrankovic, M. Graczyk-Zajac, C. Kalcher, J. Rohrer, M. Becker, C. Stabler, G. Trykowski, K. Albe and R. Riedel, *ACS Nano*, 2017, 11, 11409-11416.
- 15. Z. Wu, W. Lv, X. Cheng, J. Gao, Z. Qian, D. Tian, J. Li, W. He and C. Yang, *Chemistry-a European Journal*, 2019, **25**, 2604-2609.
- 16. A. Tolosa, M. Widmaier, B. Krüner, J. M. Griffin and V. Presser, *Sustainable Energy & Fuels*, 2018, **2**, 215-228.
- 17. K. Xia, L. Qu, X. Liu, H. Han, Z. Hou, Y. Li and S. Deng, *Applied Surface Science*, 2020, **506**.
- D. Knozowski, P. Vallachira Warriam Sasikumar, P. Madajski, G. Blugan, M. Gazda, N. Kovalska and M. Wilamowska-Zawlocka, *Nanomaterials (Basel)*, 2022, 12.