Electronic Supplementary Material

A unique dual-shell encapsulated structure design achieves stable and high-rate lithium storage of Si@a-TiO_2@a-C anode

Guang Ma*, Chong Xu (✉)*, Dongyuan Zhang, Sai Che, Yuxin Liu, Gong Cheng, Chenlin Wang, Kexin Wei, and Yongfeng Li (✉)

State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing 102249, China

E-mails: chongxu@cup.edu.cn (C.X.), yfli@cup.edu.cn (Y.L.)

* G.M. and C.X. contributed equally to this work and should be considered as co-first authors.

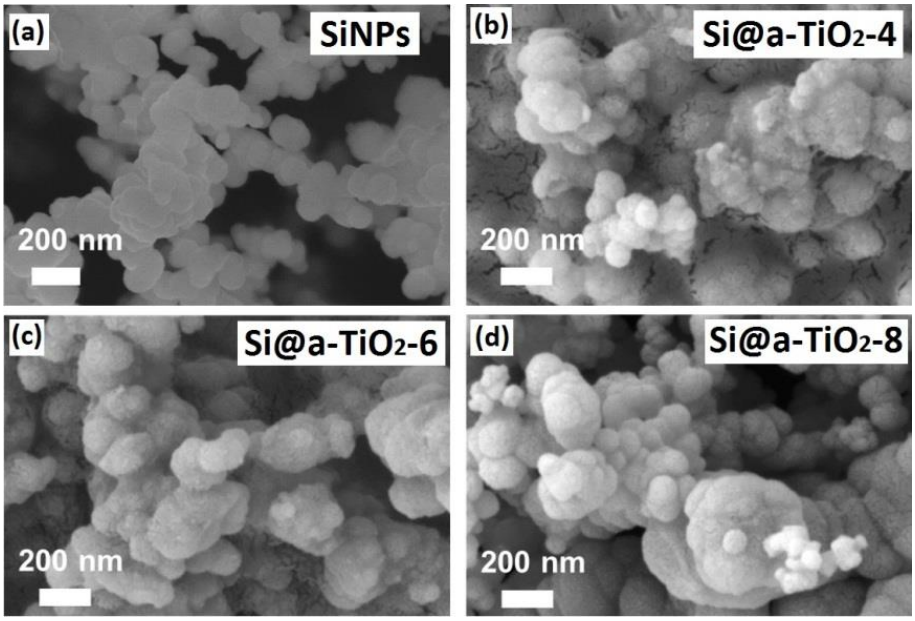

Fig. S1 SEM images of **(a)** SiNPs, **(b)** Si@a-TiO_2-4, **(c)** Si@a-TiO_2-6, and **(d)** Si@a-TiO_2-8.

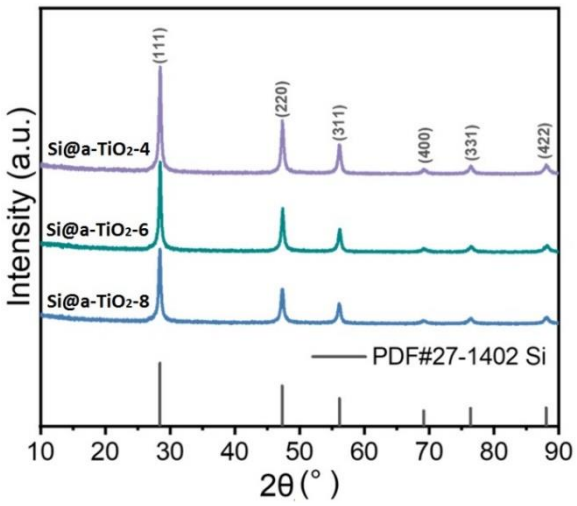

Fig. S2 XRD patterns of Si@a-TiO_2 composites.

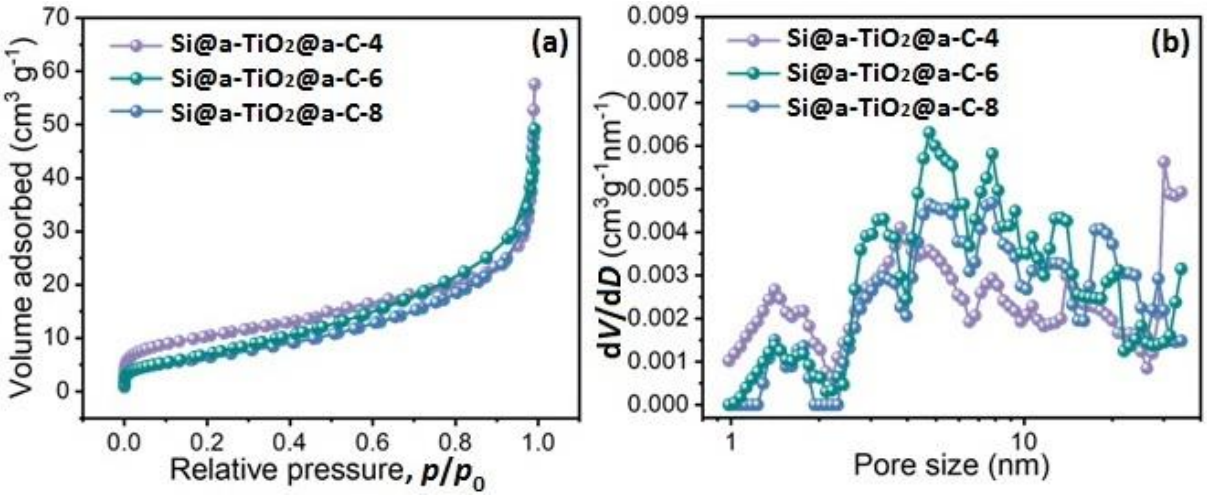

Fig. S3 (a) Nitrogen adsorption–desorption isotherms and **(b)** pore-size distributions of Si@a-TiO_2@a-C composites.

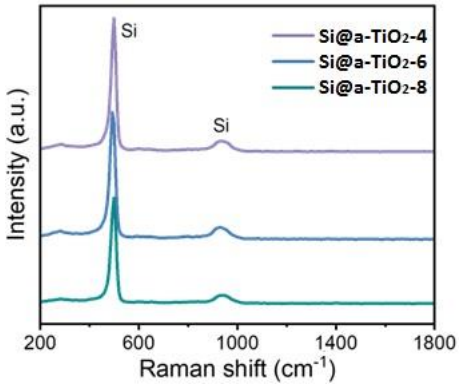

Fig. S4 Raman spectra of Si@a-TiO_2 composites.

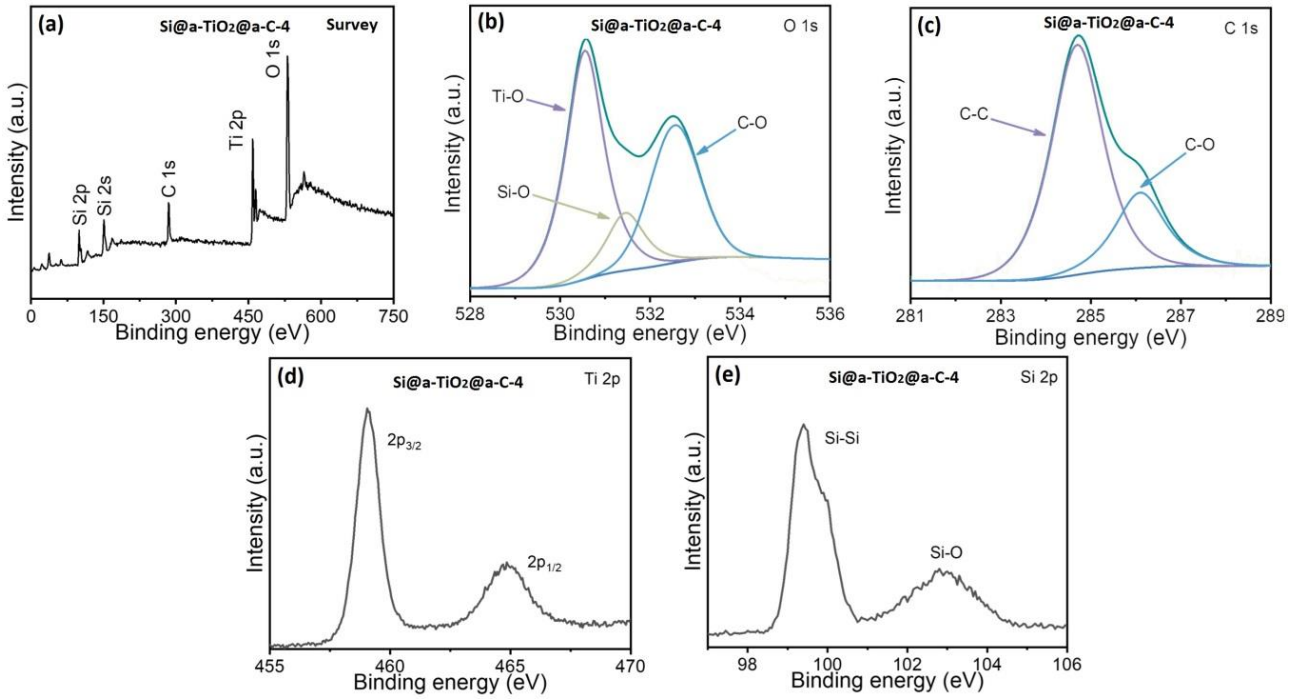

Fig. S5 (a) XPS survey spectrum of Si@a-TiO_2@a-C-4. **(b)** O 1s, **(c)** C 1s, **(d)** Ti 2p, and **(e)** Si 2p XPS spectra of Si@a-TiO_2@a-C-4.

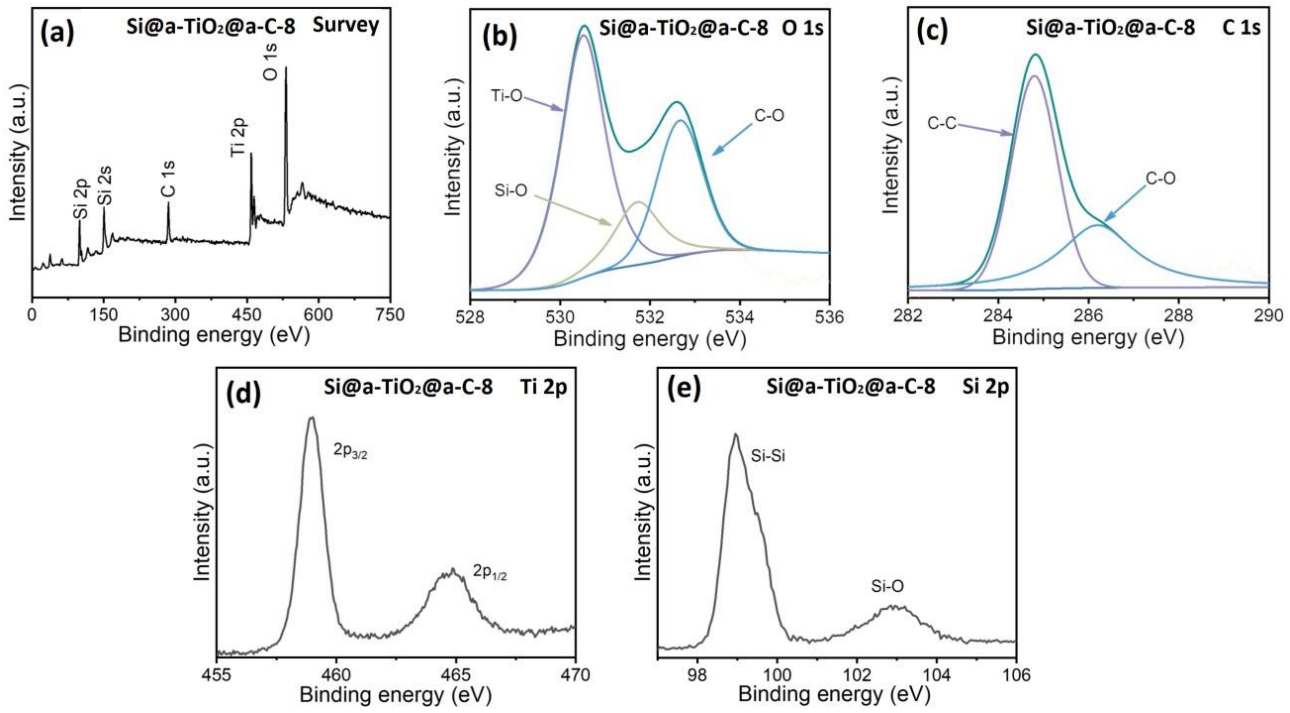

Fig. S6 (a) XPS survey spectrum of Si@a-TiO_2@a-C-8. **(b)** O 1s, **(c)** C 1s, **(d)** Ti 2p, and **(e)** Si 2p XPS spectra of Si@a-TiO_2@a-C-8.

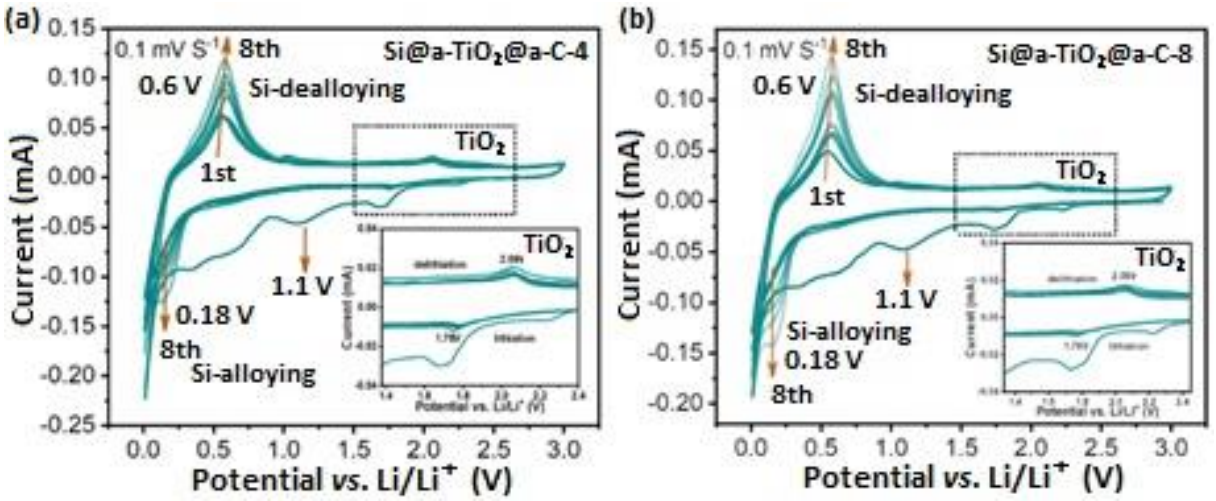

Fig. S7 (a) CV curves of Si@a-TiO_2@a-C-4 at 0.1 mV·s^{-1}. **(b)** CV curves of Si@a-TiO_2@a-C-8 at 0.1 mV·s^{-1}.

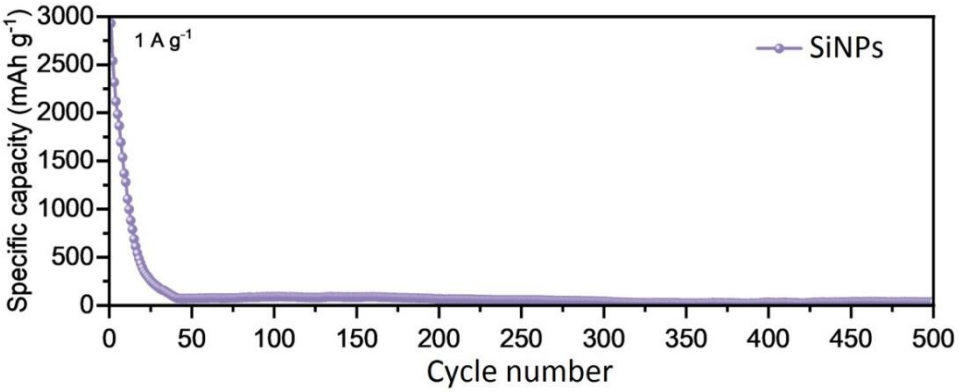

Fig. S8 Cycling performance of the SiNP composite at 1.0 A·g^{-1}.

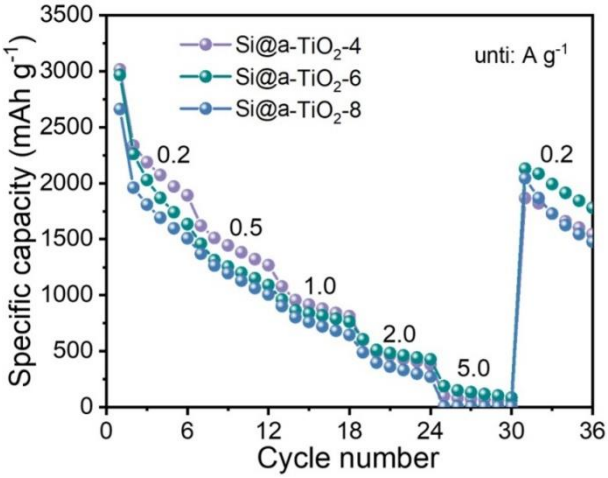

Fig. S9 Rate performance of Si@a-TiO_2 composites at different current densities.

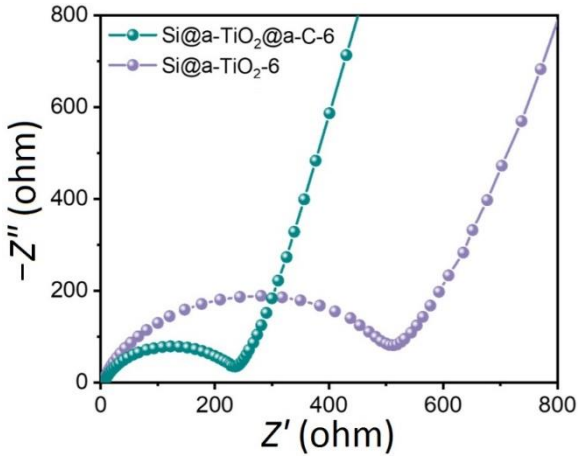

Fig. S10 Nyquist plots of Si@a-TiO_2-6 and Si@a-TiO_2@a-C-6 composites in their initial cycles.

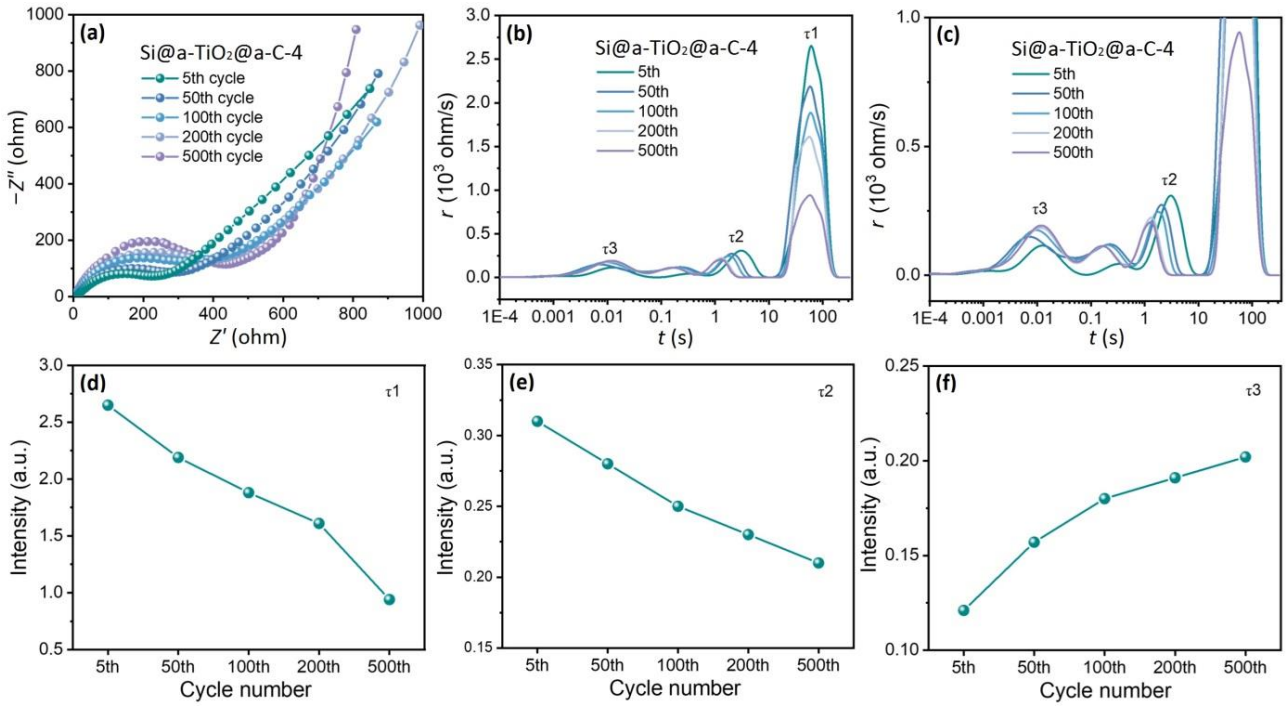

Fig. S11 (a)(b)(c) DRT analysis results obtained from EIS of Si@a-TiO_2@a-C-4 composites. **(d)(e)(f)** Peak intensity variation trends of τ_1, τ_2, and τ_3.

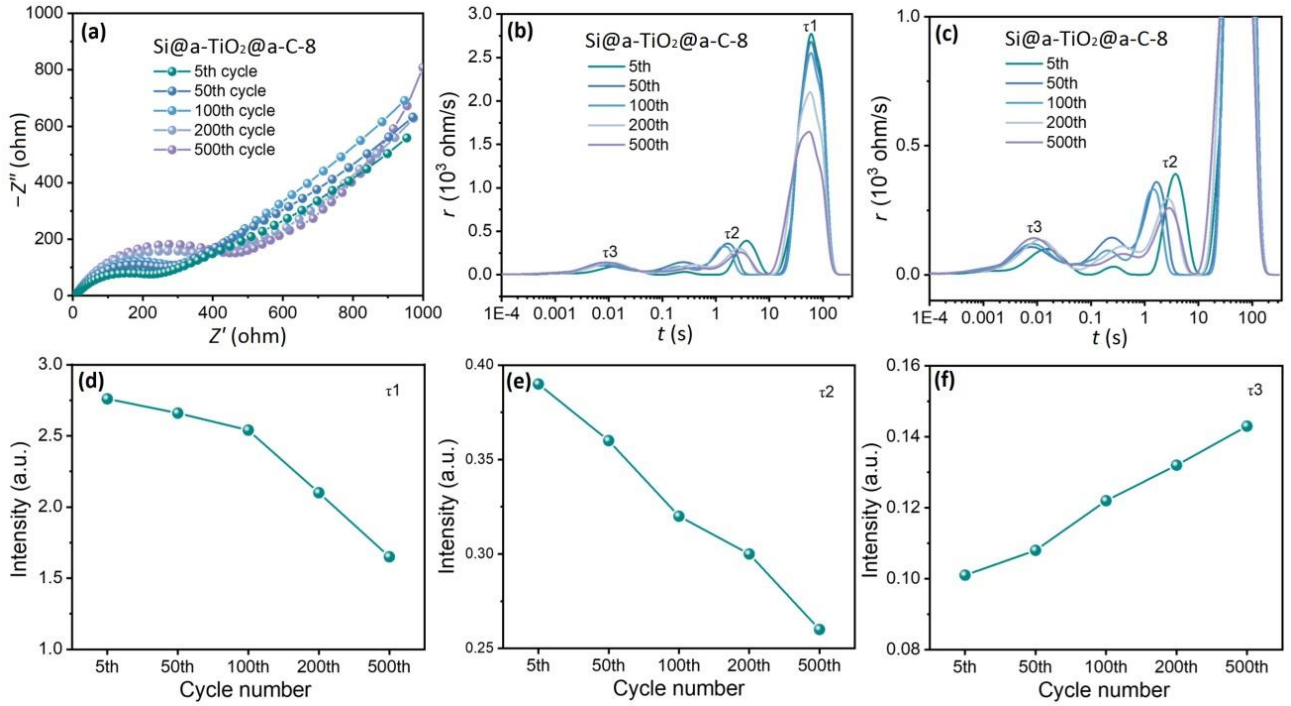

Fig. S12 (a)(b)(c) DRT analysis results obtained from EIS of Si@a-TiO_2@a-C-8 composites. **(d)(e)(f)** Peak intensity variation trends of τ_1, τ_2, and τ_3.

Table S1 Comparisons in electrochemical performances of different Si-based materials as LIBs anodes

Sb-based material	Current density/(mA·g^{-1})	Cycle number	Capacity retention after cycle/(mA·h·g^{-1})	Ref.
Si/C	210	300	783	[1]
Nanocrystal-FeSi-embedded Si/SiO_x	1000	1000	491.3	[2]
Si/SiO_x/C	1000	350	886	[3]
Si/G/GF	3579	300	445	[4]
Gr/Si/GO/C	200	100	974.5	[5]
Si/SiC/C	100	220	505.8	[6]
Si@C/rGO	200	100	935.7	[7]
(3D)Si@TiO_2@C	500	500	508.9	[8]
SA-SiTC	700	500	1122	[9]
Graphite/Si@TiO_2	500	100	511	[10]
Si@TiO_2@C	2000	100	531.5	[11]
Si@a-TiO_2@a-C	1000	500	877.1	This work

References

[1] Zheng G, Xiang Y, Xu L, et al. Controlling surface oxides in Si/C nanocomposite anodes for high-performance Li-ion batteries. Advanced Energy Materials, 2018, 8: 1801718

[2] He W, Liang Y, Tian H, et al. A facile in situ synthesis of nanocrystal-FeSi-embedded Si/SiO_x anode for long-cycle-life lithium ion batteries. Energy Storage Materials, 2017, 8: 119–126

[3] Yu R, Pan Y, Jiang Y, et al. Regulating lithium transfer pathway to avoid capacity fading of nano Si through sub-nano scale interfused SiO_x/C coating. Advanced Materials, 2023, 35: 2306504

[4] Zhu S, Zhou J, Guan Y, et al. Hierarchical graphene-scaffolded silicon/graphite composites as high performance anodes for lithium-ion batteries. Small, 2018, 14: 1802457

[5] Huang Y, Peng J, Luo J, et al. Spherical Gr/Si/GO/C composite as high-performance anode material for lithium-ion batteries. Energy Fuels, 2020, 34: 7639–7647

[6] Chen Y, Zhang J, Chen X, et al. Facile preparation of Hollow Si/SiC/C yolk–shell anode by one-step magnesiothermic reduction. Ceramics International, 2019, 45: 17040–17047

[7] Li Q, Chen D, Li K, et al. Electrostatic self-assembly bmSi@C/rGO composite as anode material for lithium ion battery. Electrochimica Acta, 2016, 202: 140–146

[8] Hou L, Xiong S, Cui R, et al. Three-dimensional porous carbon framework confined Si@TiO_2 nanoparticles as anode material for high-capacity lithium-ion batteries. ChemElectroChem, 2022, 9: 1–10

[9] Shi J, Zu L, Gao H, et al. Silicon-based self-assemblies for high volumetric capacity li-ion batteries via effective stress management. Advanced Functional Materials, 2020, 30: 1–12

[10] Vats B, Gupta R, Gupta A, et al. Enhancing Li-ion battery performance through the integration of Si@TiO_2 core–shell nanoparticles with natural graphite. ChemistrySelect, 2024, 9: e202303545

[11] Pan Q, Zhao J, Xing B, et al. A hierarchical porous architecture of silicon@TiO_2@carbon composite novel anode materials for high performance Li-ion batteries. New Journal of Chemistry, 2019, 43: 15342–15350