

Supporting Information

Phenyl-Rich Silicone Oil as a Precursor for SiOC Anode Materials in Long-Cycle and High-Rate Lithium Ion Batteries

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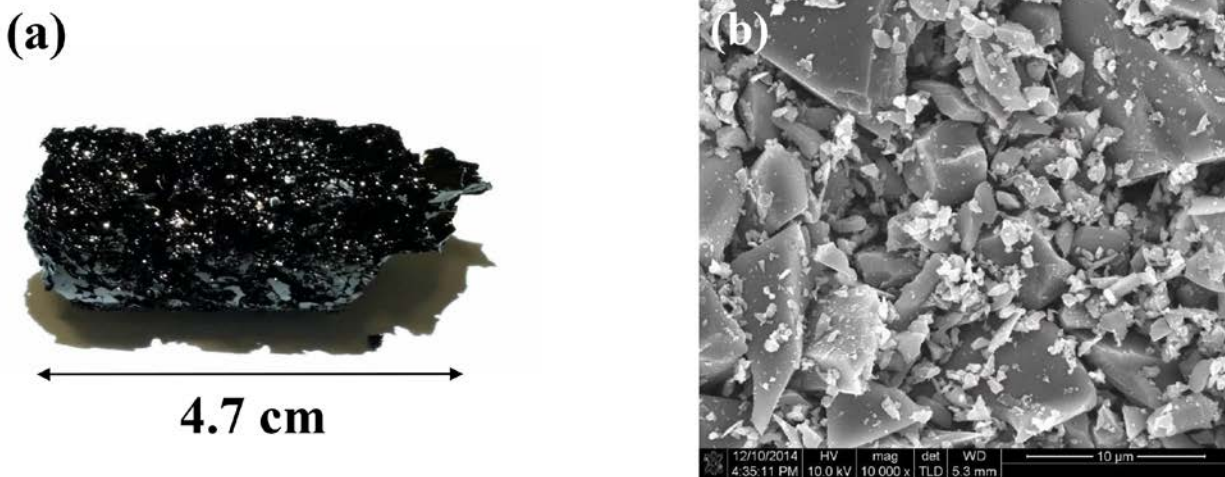


Fig. S1. (a) Digital image of the resulting SiOC after pyrolysis method. (b) SEM image of the SiOC after pulverization. The resulting SiOC after pyrolysis was a solid dense block. The SiOC was then pulverized with ball milling for 1 hour to get a fine powder.

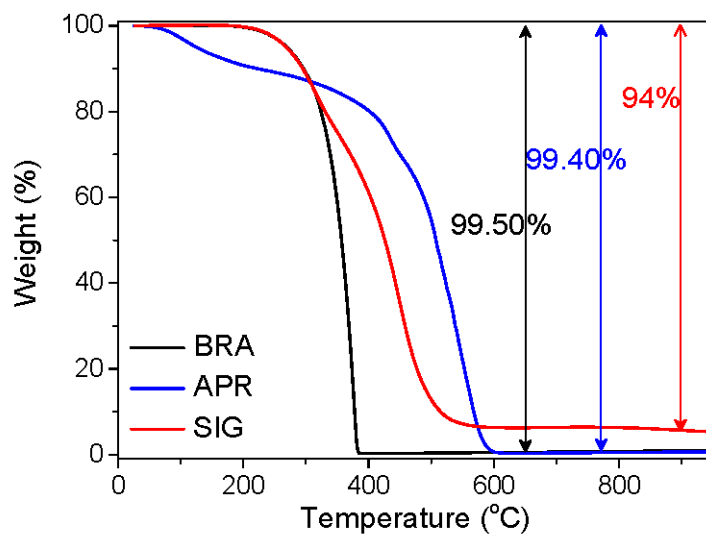


Fig. S2. Thermogravimetric analysis (TGA) of silicone oil precursors from three different suppliers: BRA, APR, SIG.

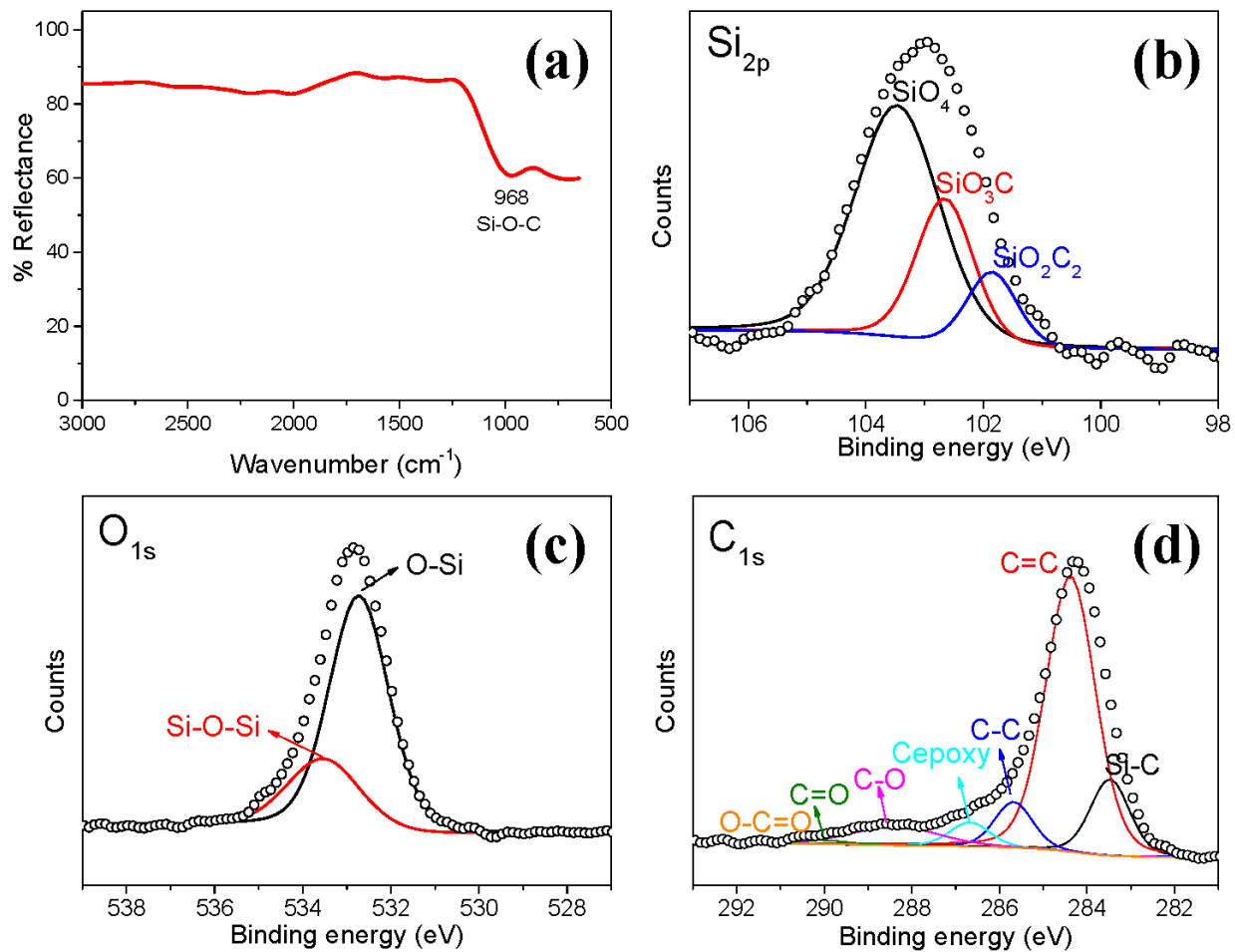


Fig. S3. Chemical bonding confirmation in SiOC by (a) FTIR and X-ray photoelectron spectroscopy (XPS) spectra of SiOC (b) Si_{2p} , (c) O_{1s} , and (d) C_{1s} .

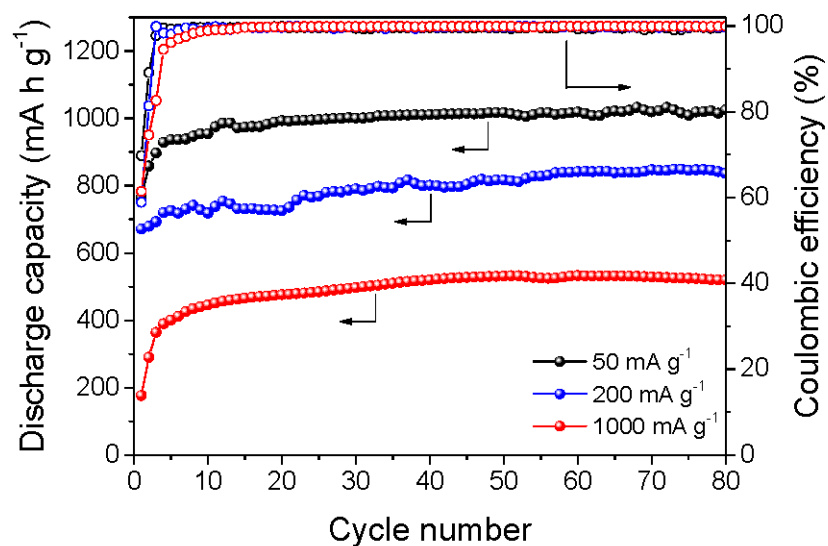


Fig. S4. Galvanostatic cycle performance of SiOC at varied current densities, 50, 200 and 1000 mA g⁻¹.

Calculation of Li⁺ Diffusion Coefficient

Lithium diffusion coefficient (D_{Li^+}) within SiOC anode material is calculated based on the Randles-Sevcik equation:

$$i = 2.69 \times 10^5 n^{1.5} A D_{Li^+}^{0.5} C_{Li} \nu^{0.5}$$

where, i is the peak current (A), n is the number of electrons per species reaction (1 for lithium ion), A is the electrode surface area (1.131 cm²), D_{Li^+} is the lithium ion coefficient within the SiOC anode material, ν is the potential scan rates and C_{Li} is the lithium concentration in electrolyte (10⁻³ mol cm⁻³). The value of i and $\nu^{0.5}$ can be obtained from the cyclic voltammetry in Fig. S5a. The relationship of i and $\nu^{0.5}$ is expressed in the linear equation as shown in Fig. S5b. Further, the gradient obtained in Fig. S5b is used to determine the value of lithium diffusion coefficient (D_{Li^+}) within SiOC.

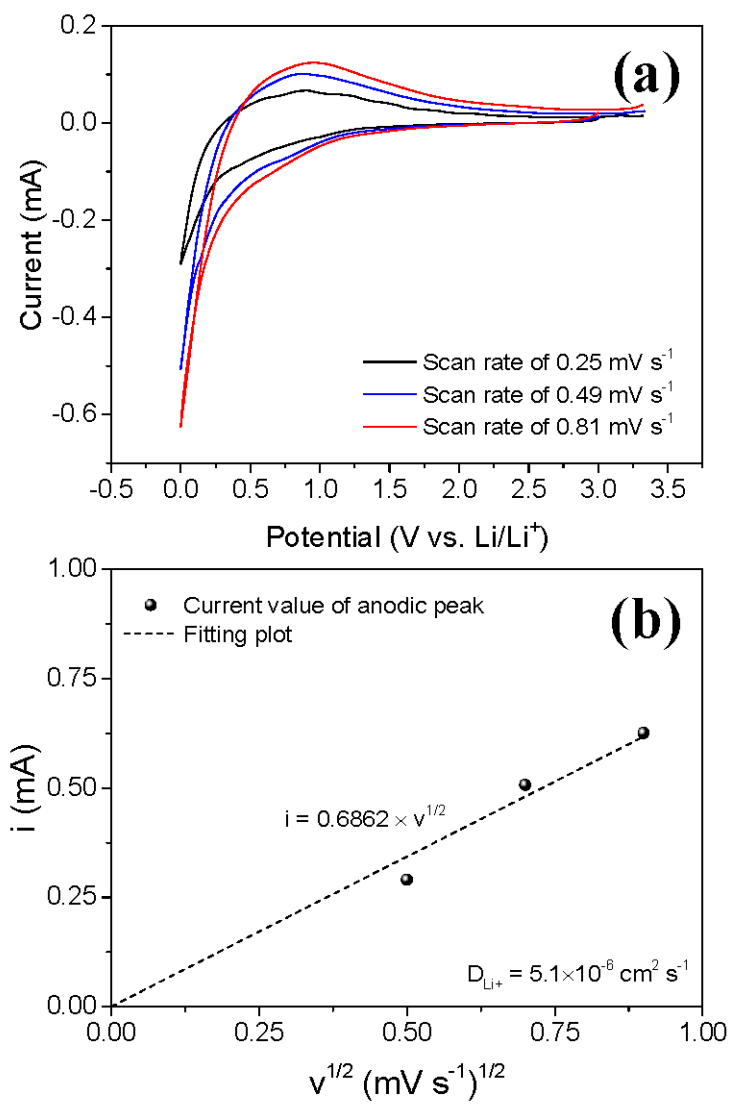


Fig. S5. (a) Cyclic voltammety profile of SiOC at varied scan rates. (b) Plot of the peak current and square root of the scan rate of the SiOC anode materials.

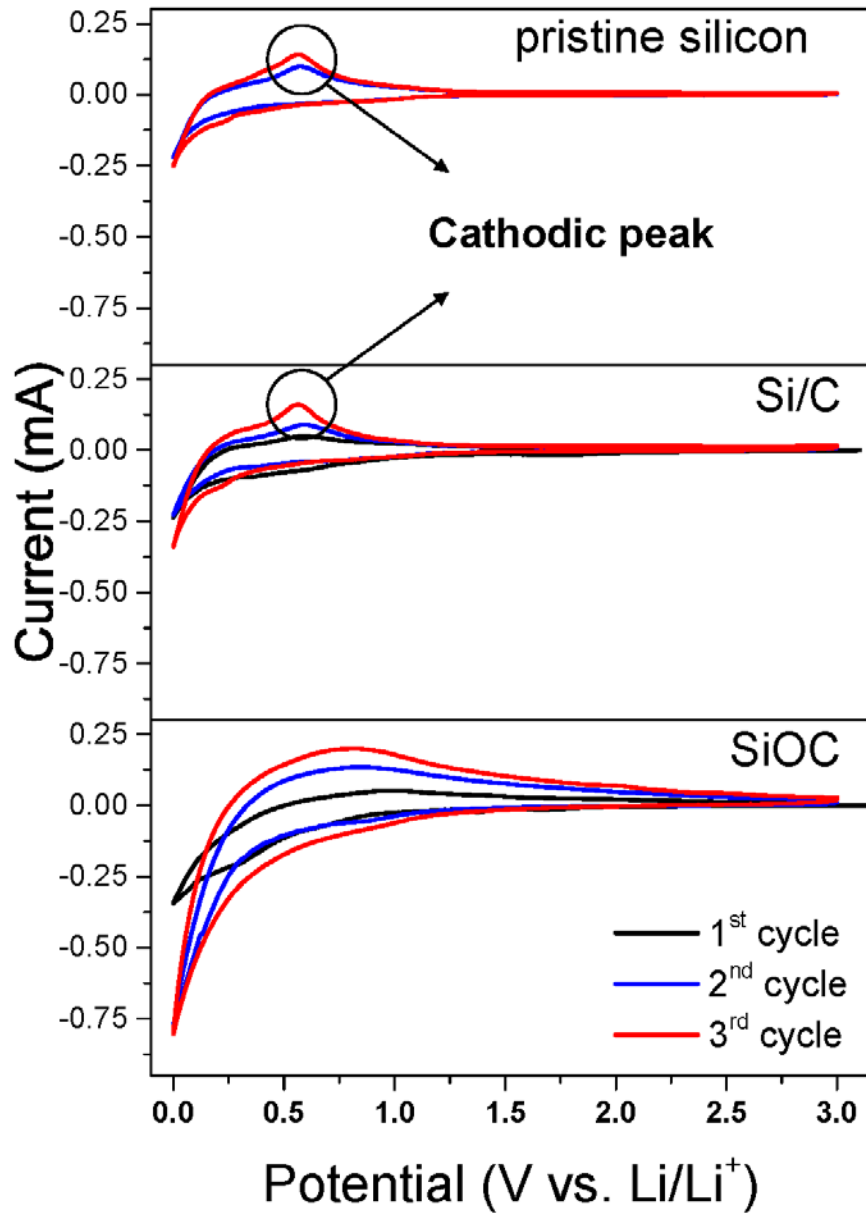


Fig. S6. Cyclic voltammetry (CV) profiles of (a) pristine Si microparticle, (b) Si/C composite, and (c) SiOC at the scan rate of 0.2 mV s^{-1} and cut-off voltage of 0.001 – 3.0 V.

Table S1. Material composition and mass ratio (%) of SiOC by X-ray fluorescence (XRF) analysis.

| No | Component | Result (mass %) |
|----|-----------|-----------------|
| 1 | Si | 59 |
| 2 | Fe | 0.0033 |
| 3 | Ni | 0.0061 |
| 4 | Zr | 0.0166 |
| 5 | C | 39.9 |
| 6 | H | 1.1 |

Material composition of SiOC mostly consists of Si and C (6:4). Meanwhile, the Fe, Ni, and Zr might come from the trace impurities in the precursor and from the pulverization process using ball milling.

Table S2. Electrochemical performance of SiOC anode materials in lithium ion batteries prepared by using different precursors

| Published Year | SiOC Precursor | Current density | Discharge capacity | | Reference |
|----------------|---|-------------------------------|--------------------|-------------------------|------------------|
| | | | | (mA h g ⁻¹) | |
| - | Silicone oil | 50 mA g⁻¹ | 1050 | 80 | this work |
| | | 200 mA g⁻¹ | 800 | 250 | this work |
| | | 1000 mA g⁻¹ | 520 | 80 | this work |
| 2015 | Polyhydridomethylsiloxane (PHMS) + divinylbenzene (DVB) + platinum divinyltetramethyldisiloxane | 360 mA g ⁻¹ | 600 | 50 | [1] |
| 2013 | polyorganosiloxane (Polyramic® RD-684) | 37 mA g ⁻¹ | 666 | 10 | [2] |
| 2012 | polyorganosiloxane (Polyramic® RD-684) | 37 mA g ⁻¹ | 532 | 10 | [3] |
| 2012 | polyhydridomethylsiloxane (PHMS) | 18 mA g ⁻¹ | 190 | 10 | [4] |
| 2011 | Tetramethyl-tetravinylcyclotetrasiloxane + dicumyl peroxide | 100 mA g ⁻¹ | 637 | 60 | [5] |
| 2009 | Graphene oxide + polyhydrodimethylsiloxane (PHMS) | 40 mA g ⁻¹ | 357 | 20 | [6] |
| 2005 | polysiloxanes | 0.15 mA cm ⁻² | 550 | 10 | [7] |
| 1999 | pitch + polyphenylmethyl silane | - | 500 | 2 | [8] |
| 1994 | polymethylphenylsiloxane (Dow 710 fluid) | 74 mA g ⁻¹ | 380 | 25 | [9] |

References

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