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Supplementary Information

Multifunctional TiO_2 coating for SiO anode in Li-ion batteries

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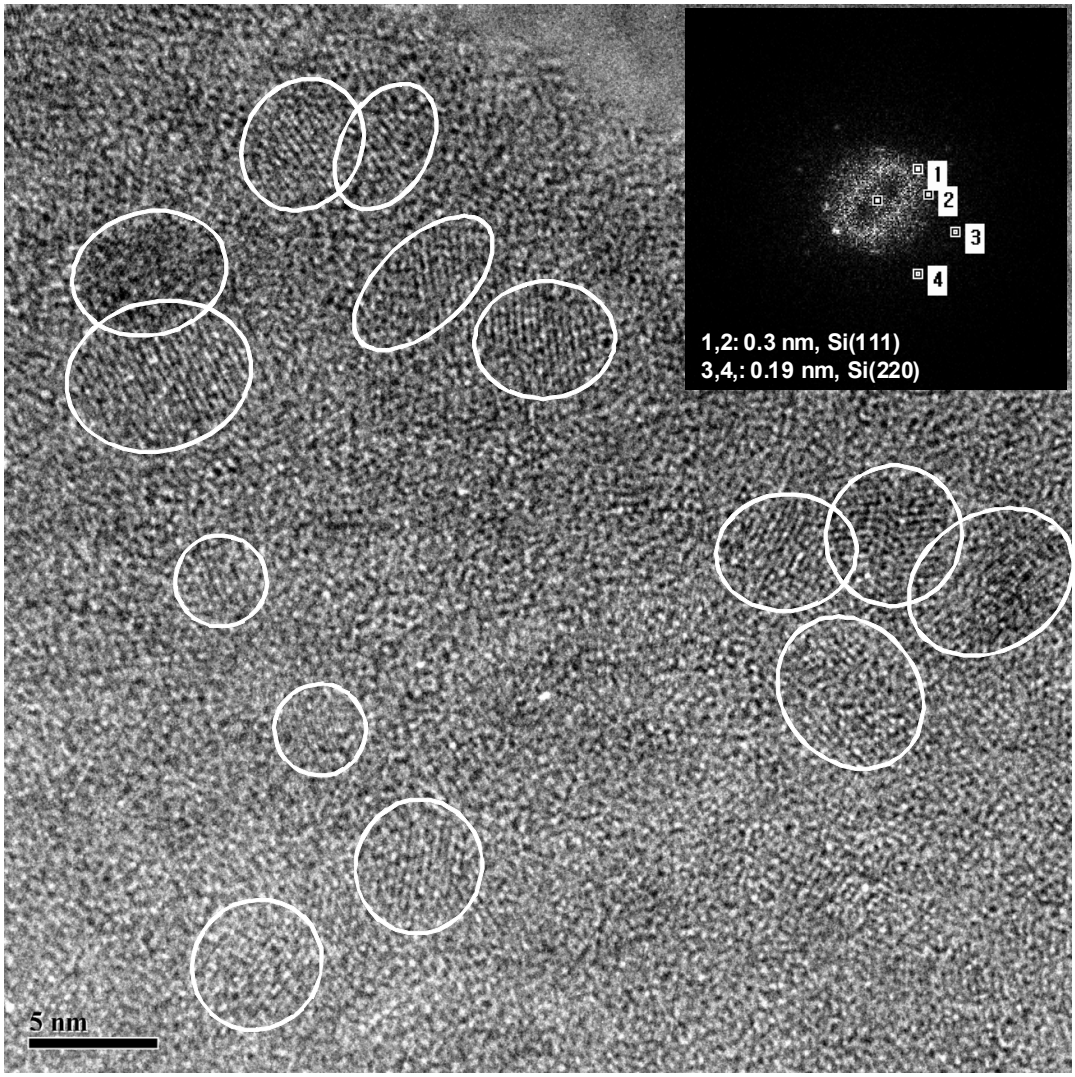

Fig. S1 HRTEM image and SAED pattern of bare SiO material

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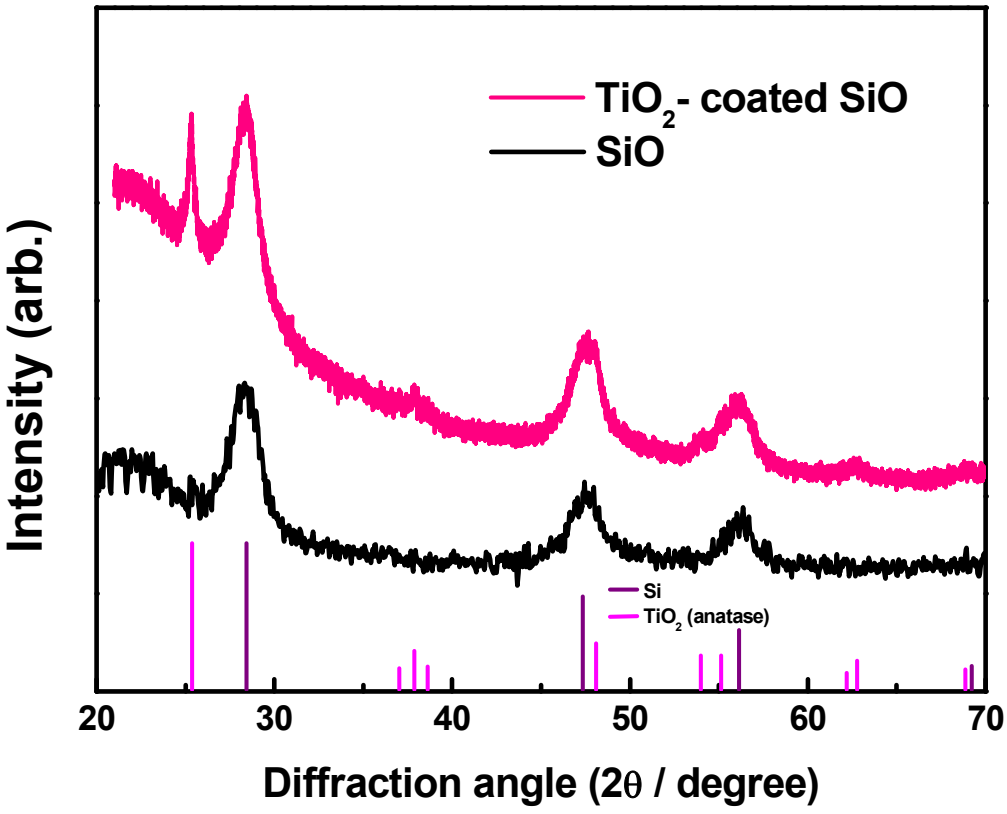

Fig. S2 XRD patterns of SiO and TiO_2-coated SiO materials

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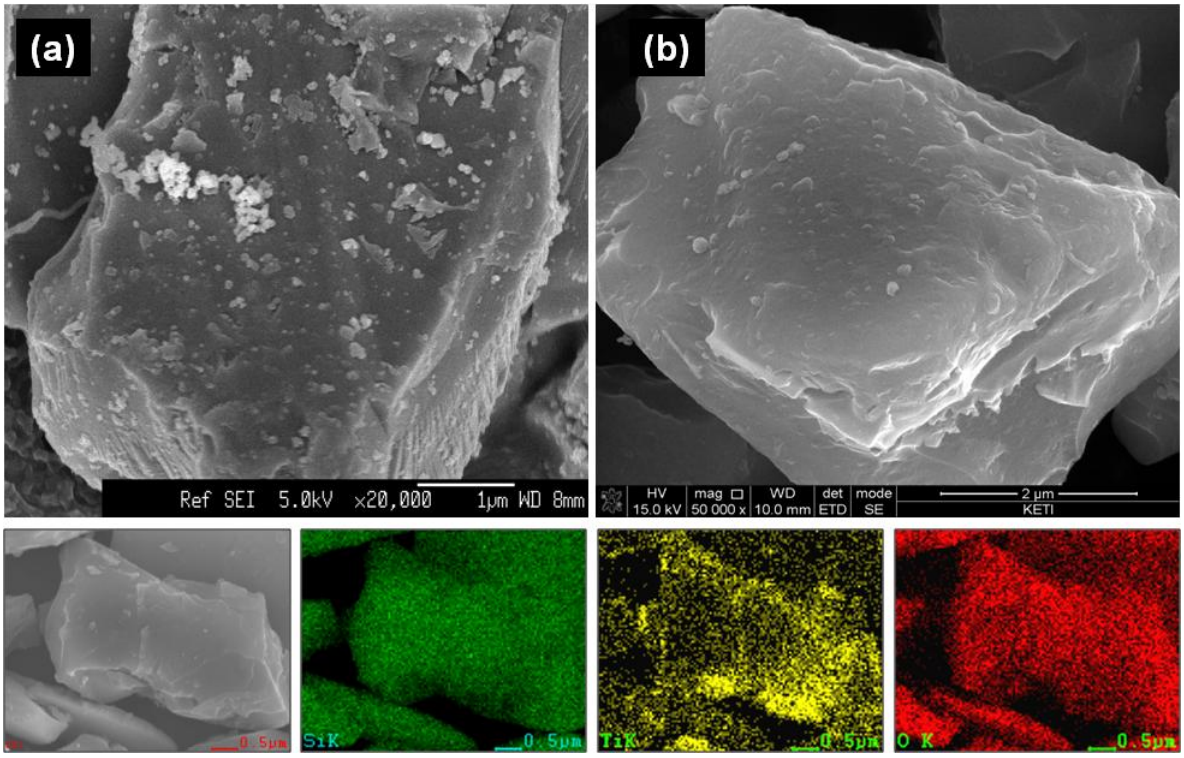

Fig. S3 SEM image of (a) bare SiO and (b) TiO_2-coated SiO. SEM–EDS elemental mapping of the TiO_2-coated SiO are also shown in below.

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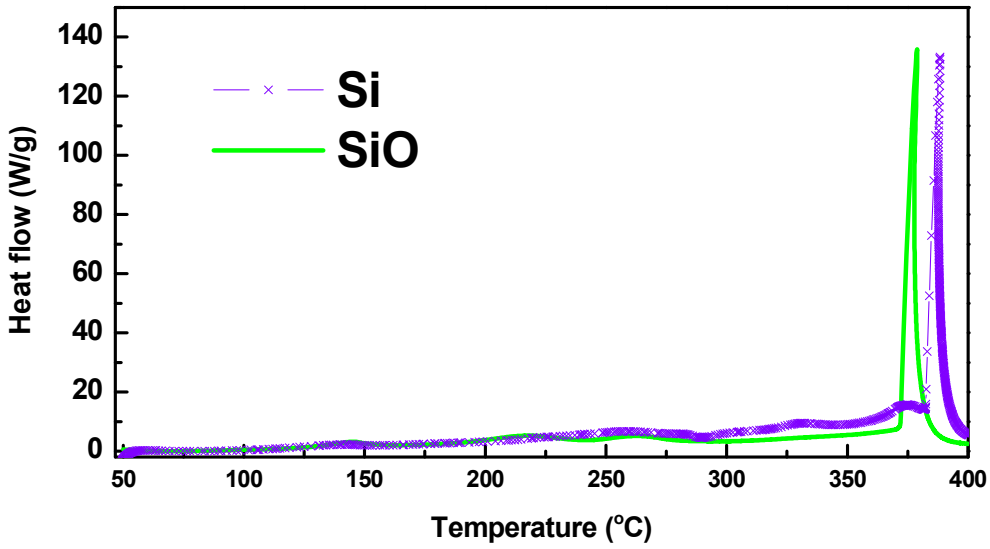

Fig. S4 DSC profiles of Si and SiO after fully-lithiated (100% SOC) at the first cycle

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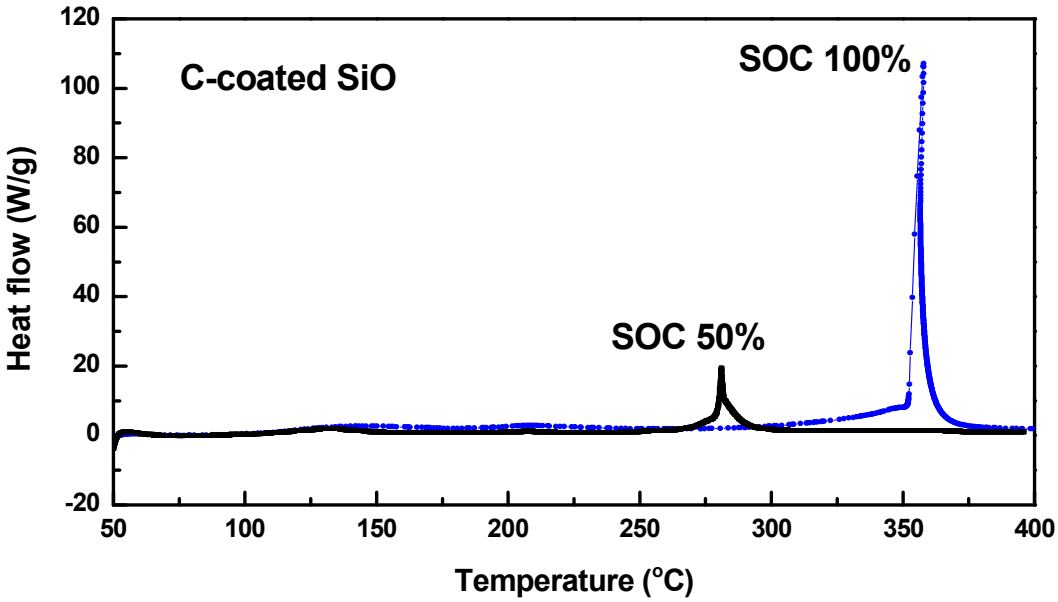

Fig. S5 DSC profiles of carbon-coated SiO at different SOC levels

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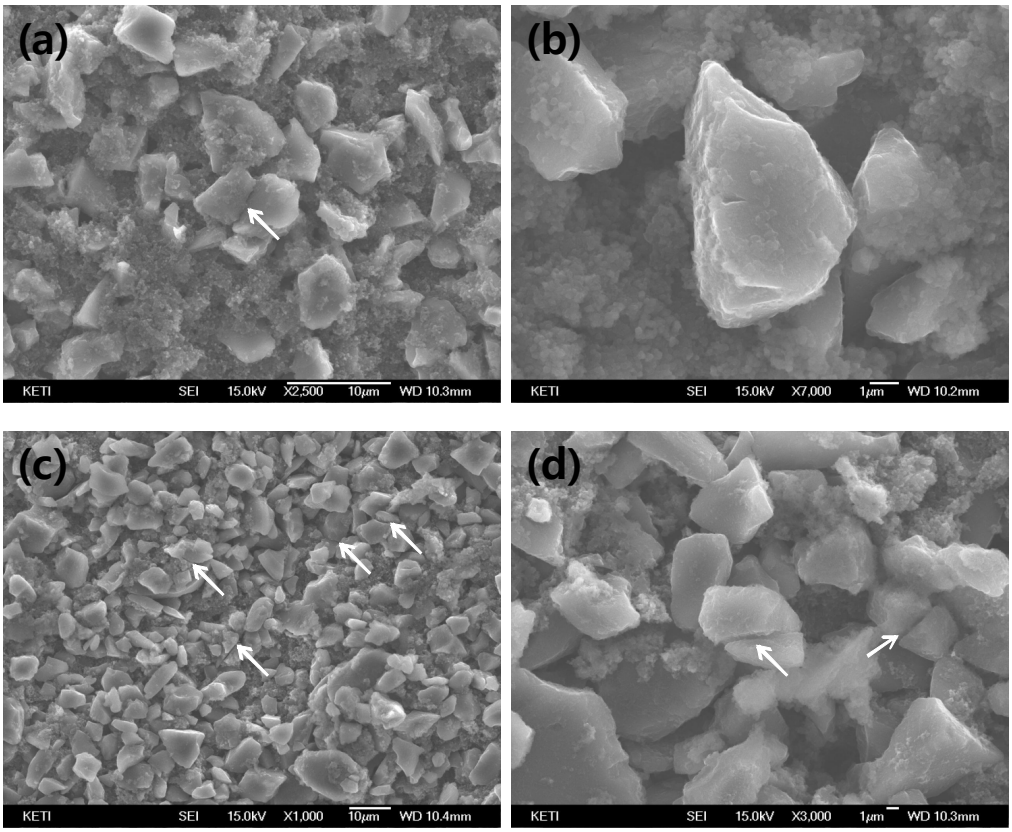

Fig. S6 SEM images of (a,b) TiO_2-coated SiO and (c,d) bare SiO electrodes after 1st discharge

Mechanical stability of the TiO_2 coating layers as well as the TiO_2-coated SiO particles after the 1st discharge was investiaged. Fig. S6 shows SEM images of the Li-inserted TiO_2-coated SiO and bare-SiO particles. Although a little fracture was found in some particles (less in the TiO_2-coated SiO), most of the particles sustain their initial morphology. Concerning the TiO_2-coating layer itself, no mechanical degradation (cracks) was found.

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Table S1 Design parameters and the simulated results of single-stack-modeled full cells

Design parameters	TiO_2-coated SiO	bare SiO	graphite
Cathode ($LiCoO_2$)			
Charge capacity / mAh g^{-1} *	158	←	←
Discharge capacity / mAh g^{-1}	153	←	←
Initial Coulombic efficiency / %	96.8	←	←
Ratio of active material / %	96	←	←
Ratio of binder / %	2	←	←
Ratio of carbon black / %	2	←	←
Electrode density / g cm^{-3}	3.7	←	←
Charge capacity per unit area / mAh cm^{-2}	3.6	←	←
Loading level / mg cm^{-2}	23.8	←	←
Electrode thickness / μm	64	←	←
Anode			
Charge capacity / mAh g^{-1}	1757	2260	384
Discharge capacity / mAh g^{-1} **	1265	1202	362
Initial Coulombic efficiency / %	72	53	94
Ratio of active material / %	80	←	90
Ratio of binder / %	10	←	10
Ratio of carbon black / %	10	←	0
Electrode density / g cm^{-3}	1.1	←	1.5
Others			
N/P ratio	1.1	←	←
Cu thickness / μm	10	←	←
Al thickness / μm	20	←	←
Separator thickness / μm	16	←	←

* 4.2 V for charging voltage of full cells

** 2.0 V discharge voltage for the SiO-based/LCO full cell, 3.0 V for the graphite/LCO full cell

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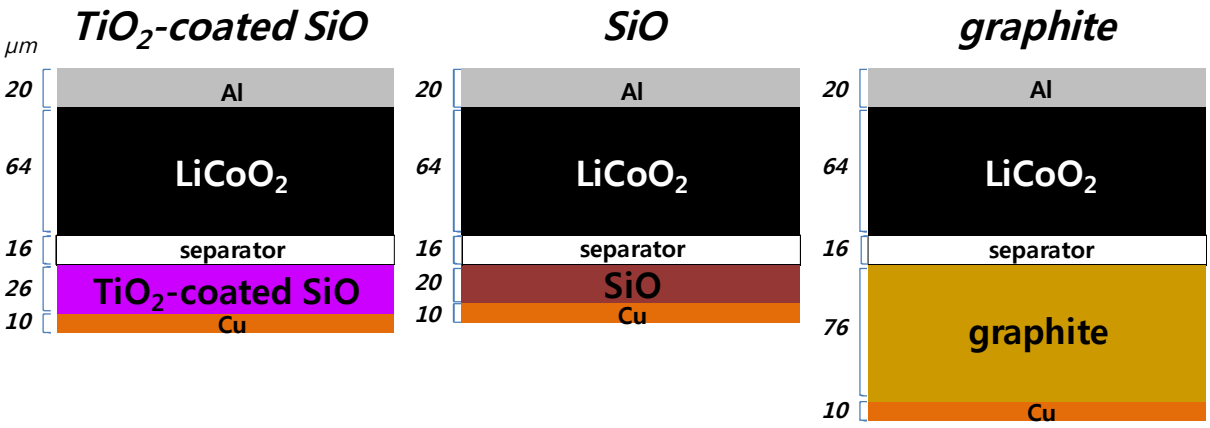
Table S1 *(continue)*

Simulated results	TiO_2-coated SiO	bare SiO	graphite
Anode			
Loading level / mg cm^{-2}	2.82	2.19	11.47
Electrode thickness / μm	26	20	76
Single-stacked full cells			
Discharge capacity per unit area / mAh cm^{-2}	2.594	1.916	3.396
Volume of stack / cm^{-3}	0.01358	0.01301	0.01866
Volumetric capacity / Ah L^{-1}	191	147	182
Operating mid-voltage / V	3.58	3.58	3.7
Volumetric energy density / Wh L^{-1}	684	527	673



Simulation of volumetric energy density and voltage profile was carried under the following conditions.

1) 1-dimenional single-stacked full cell (including Al, Cu substrates, see the above schematic views) was considered as a model structure for simulation.
2) Charging voltage of full cells; 4.2 V
3) Discharge cut-off voltage for the full cells employing SiO and TiO_2-coated SiO is 2.0 V,

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corresponding to ca. 2.0 V vs Li/Li^+ cut-off potential for the anodes in the half-cells. Discharge cut-off voltage for the full cell employing graphite is 3.0 V.

4) Loading of cathode
   - Loading of cathode composite film ($LiCoO_2$+carbon black+binder) was fixed at 23.8 mg cm^{-2}, corresponding to 3.6 mAh cm^{-2} capacity for charging.
5) Electrode density of anodes
   - 1.1 g cm^{-3} electrode density was employed for SiO and TiO_2-coated SiO anode, which is the value of the less roll-pressed electrode to buffer volume expansion of the SiO-based anodes. (Their maximum electrode densities are ca. 1.3 g cm^{-3} in which the volume expansion of the anodes exceed 100%, observed experimentally)
   - 1.5 g cm^{-3} electrode density was applied for graphite anode, which is normally found in the commercial Li-ion batteries.
6) Loading and thickness of anodes
   - By N/P ratio (1.1) and the electrode densities, loading and thickness of the anodes were determined.
7) Voltage profile and energy density
   - Voltage profiles and volumetric energy densities of the full cells were obtained from the experimental voltage profiles of anode and cathode in their half-cells, using the OriginPro 8 SR4 program.