Supporting Information

Porous MoS_2@C hetero shell with Si yolk structure with improved lithium transport properties and superior cycle stability

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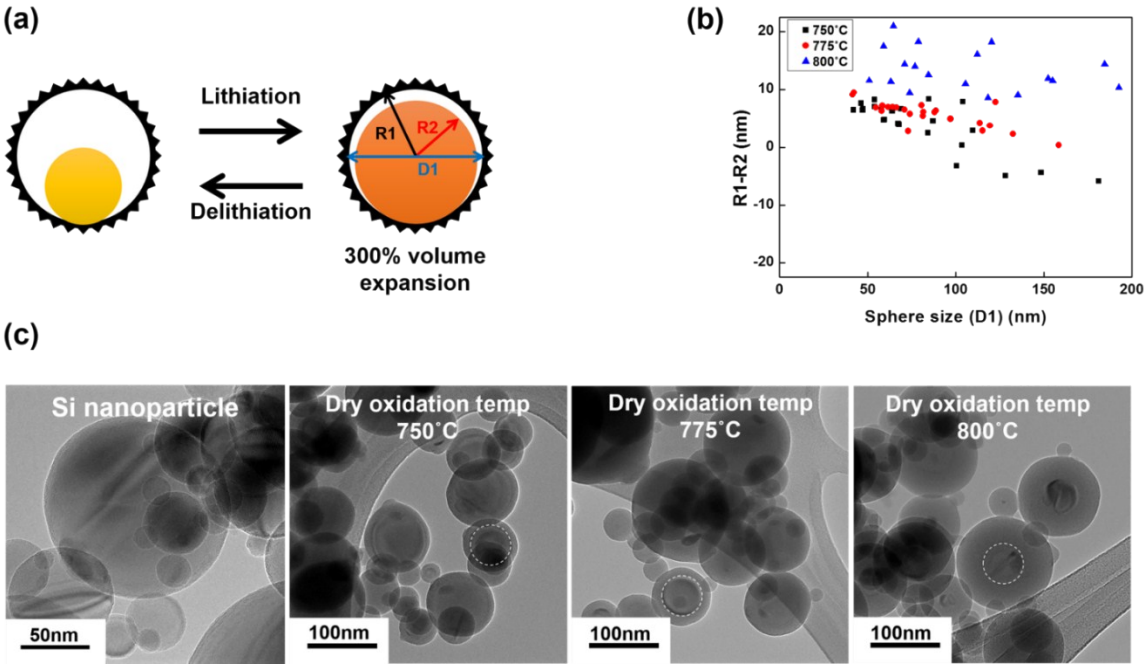

Figure S1. (a) Illustration of Si core volume expansion of SCM yolk-shell structure. (b) The Si volume expansion calculation scatter diagram for various dry oxidation temperatures. (c) HR-TEM image of Si nanoparticles and Si@SiO_2 nanoparticles for various the dry oxidation temperatures.

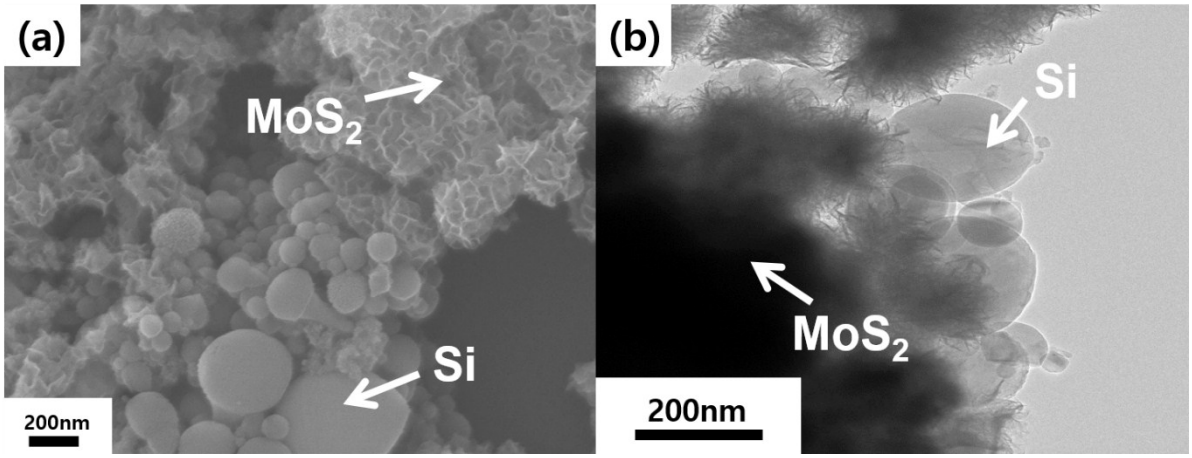

Figure S2. (a) FE-SEM image, (b) HR-TEM image of synthesized of Si/MoS2 nanoparticles without a PDA coating on the $Si@SiO_2$ surface.

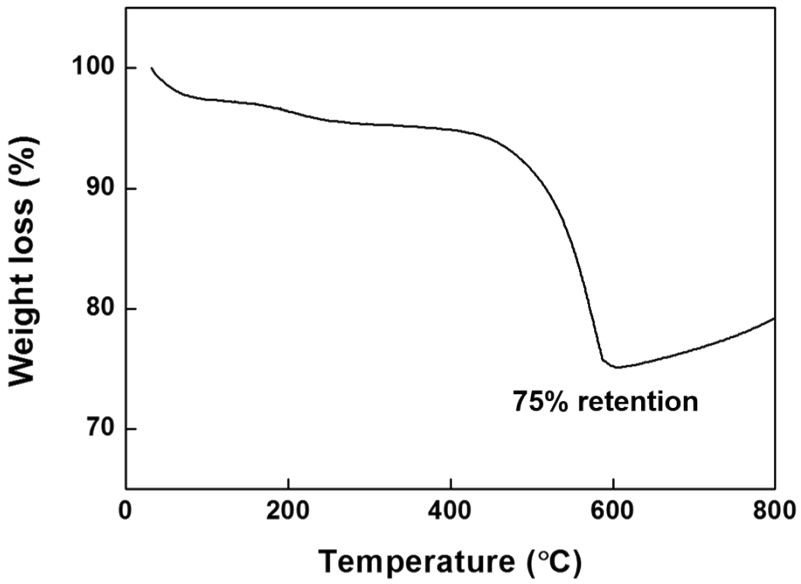

Figure S3. Thermogravimetric Analysis (TGA) results of the Si@C sample. The sample was heated under the air.

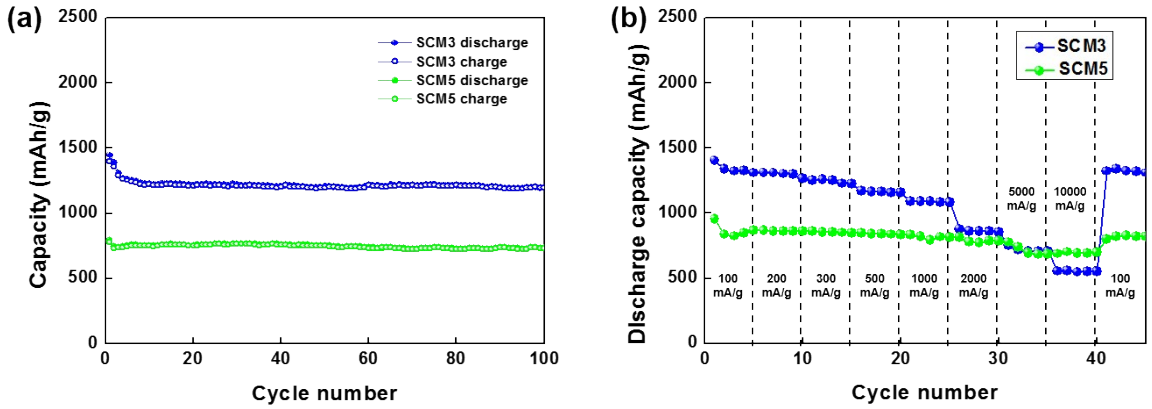

Figure S4. (a) Cycling performance and coulombic efficiency of SCM3 and SCM5 based on various current densities: 1st = 100 mA/g, 2nd = 200 mA/g, and 3rd and following = 500 mA/g. (b) Rate capabilities of SCM3, SCM5.

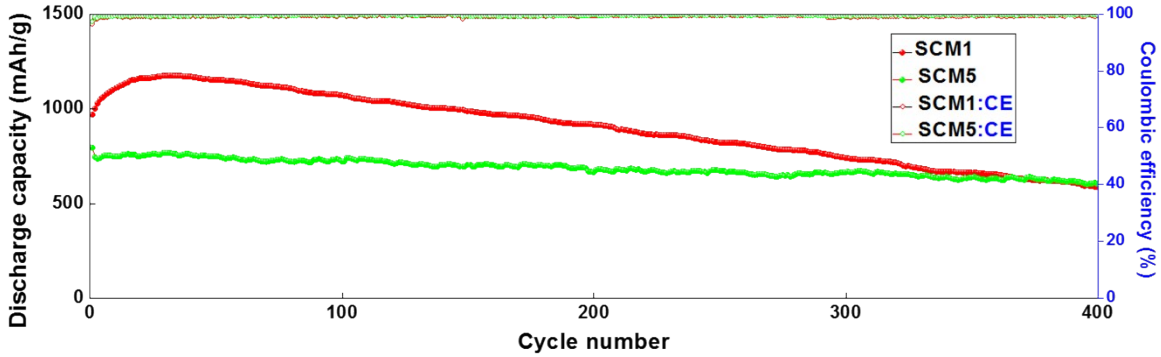

Figure S5. Long-term cyclic test of SCM1, SCM5 at a current density of 2000mA/g.

To further check electrochemical stability effect according to MoS_2 shell thickness, we measured the long term cyclic test injected high current density of 2,000 mA/g. In the initial 30 cycles, the SCM1 capacity value is increased because of the silicon activation.[1] After then, the capacity is decreased because of the thin shell structure. However, in the SCM5, the initial capacity increase such as SCM1 doesn't show and the capacity retention is increased because of the thick shell structure.

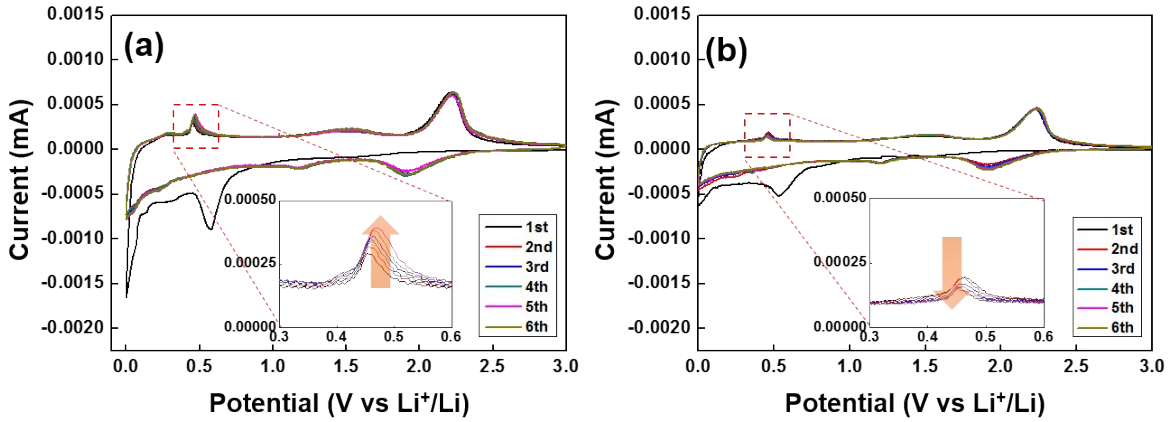

Figure S6. Cyclic voltammetry of (a) Si@C, (b) SCM1 at a scan rate of 0.1 mV/s.

To explain the decrease of capacity value according to the shell thickness. We additionally measured the cyclic voltammetry of SCM3, SCM5. In SCM3 (figure S6a), the cathodic peak intensity around 0.5 V doesn't high compared to the SCM1 (figure 4b) although the peak slightly increased. In SCM5 (figure S6b), the peak intensity around 0.5 V decreased rather. Those result show close correlation between the shell thickness and capacity value & retention.

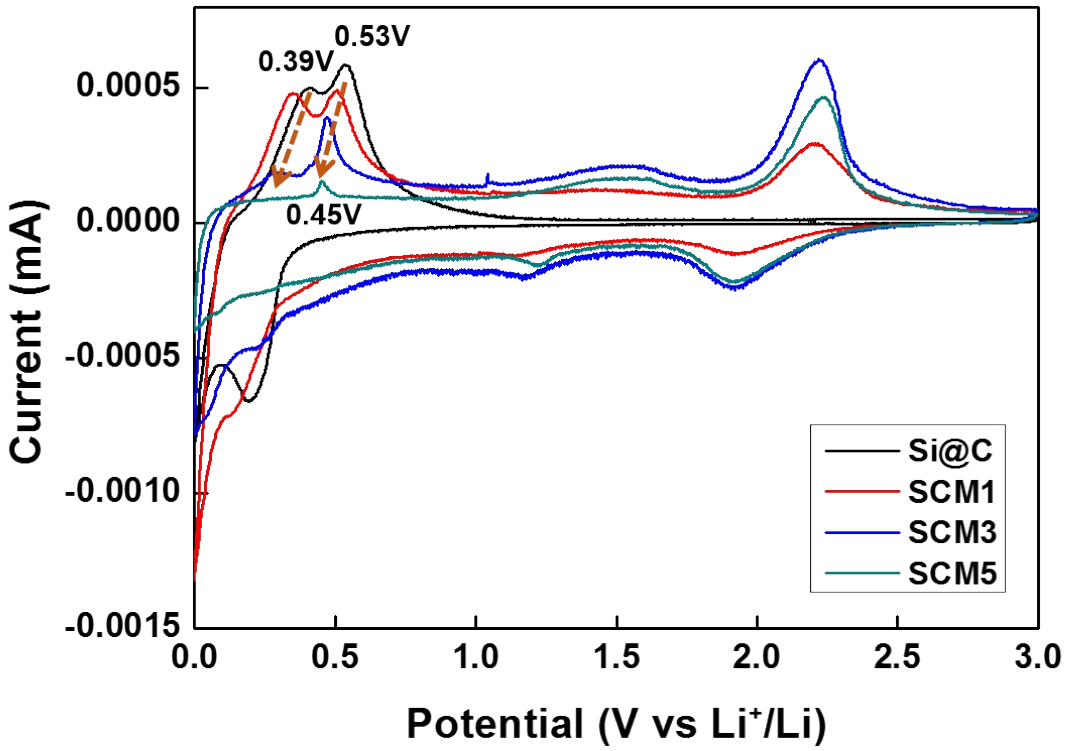

Figure S7. Cyclic voltammetry at 5th cycle of Si@C, SCM1, SCM3 and SCM5 at a scan rate of 0.1 mV/s.

Based on these basic cyclic voltammetry of Si@C, SCM1, SCM3 and SCM5, we plot the 5th CV curve of Si@C, SCM1, SCM3 and SCM5 for more detailed electrochemical analysis. As shown in the CV curve, the Si de-alloying reaction at cathodic scan is gradually decreased and the peak corresponding to the reaction is shifted to low voltage. It suggests that the Si reaction with Li ion goes gradually down as the thickness of MoS_2 layer increases.[2]

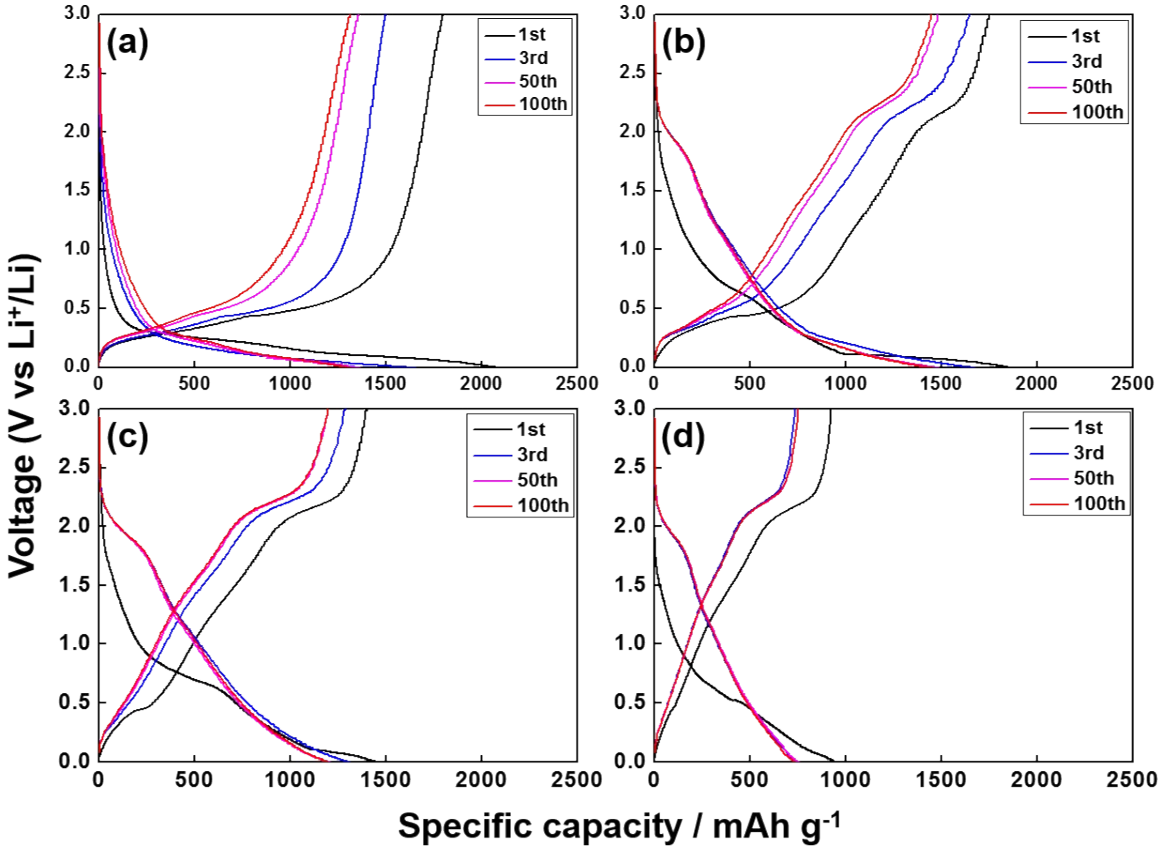

Figure S8. Charge-discharge profile of (a) Si@C, and SCM electrodes: (b) SCM1, (c) SCM3, and (d) SCM5.

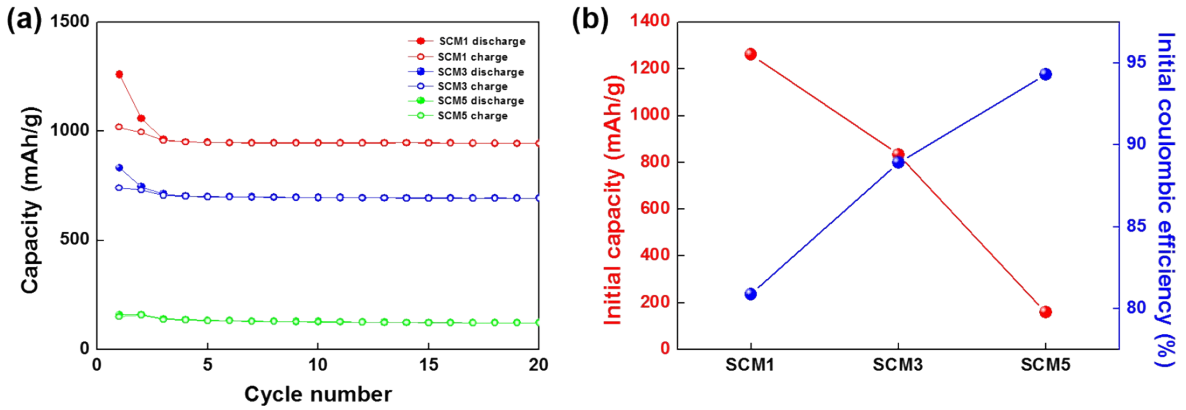

Figure S9. (a) Cycling performance and (b) initial coulombic efficiency of SCM1, SCM3 and SCM5 at 0.01 ~ 1.5V (Li/Li^+) range based on various current densities: 1^{st} = 100 mA/g, 2^{nd} = 200 mA/g, and 3^{rd} and following = 500 mA/g.

For detail analysis of MoS_2 lithium transport property, we measured electrochemical cycling test at the voltage range 0.01 ~ 1.5V. The cyclic performance result is very similar with the cycling performance at the voltage range 0.01 ~ 3.0V. From the analysis, the SCM5 electrode didn't react with lithium ion (the capacity value shows only 150mAh/g). We clearly find that there is critical point of MoS_2@C shell thickness for silicon reaction with lithium ion. The maximum shell thickness of MoS_2@C shell for silicon reaction with lithium ion is 15.2nm. The silicon doesn't react with lithium ion above 15.2nm.

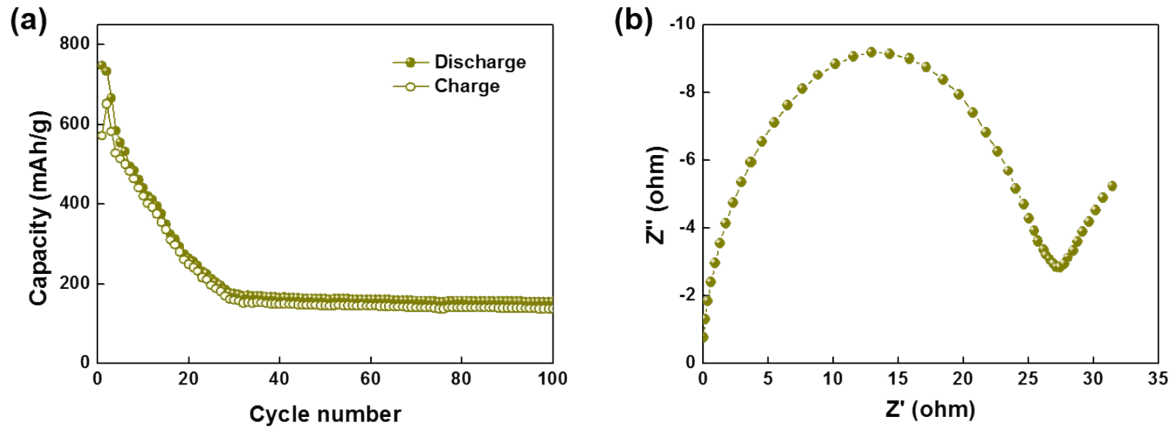

Figure S10. (a) Cycling performance and (b) EIS plot of bare MoS_2 nanoparticle based on various current densities: 1st = 100 mA/g, 2nd = 200 mA/g, and 3rd and following = 500 mA/g.

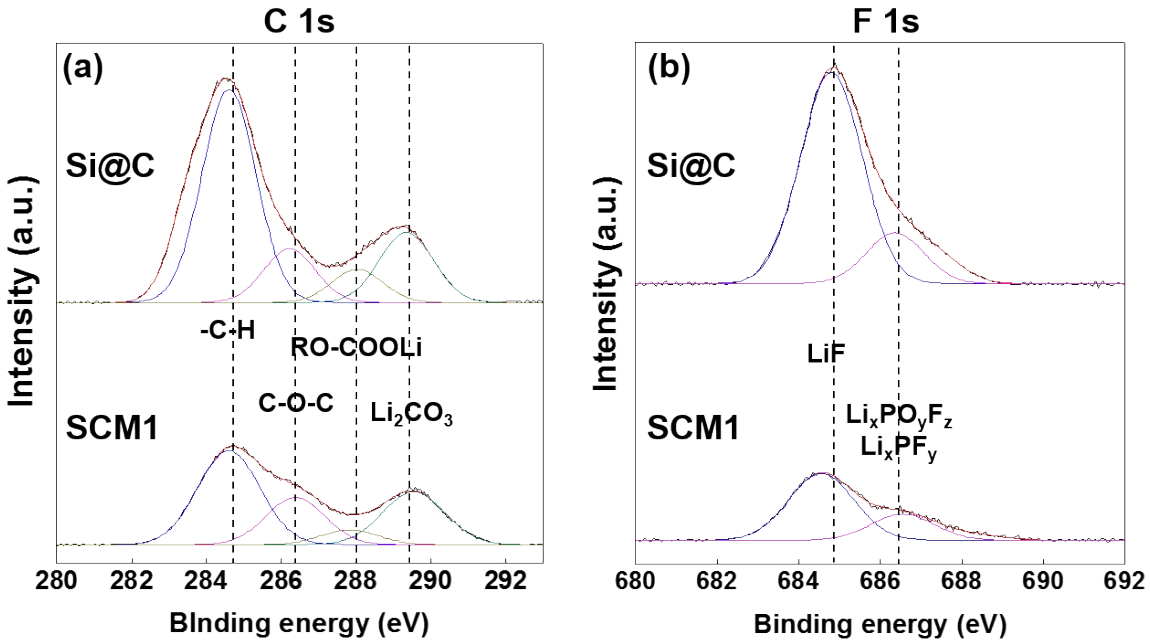

Figure S11. XPS spectra of Si@C and SCM1 electrodes of (a) C 1s (b) F 1s after 100 cycles based on various current densities: 1st = 100 mA/g, 2nd = 200 mA/g, and 3rd and following = 500 mA/g.

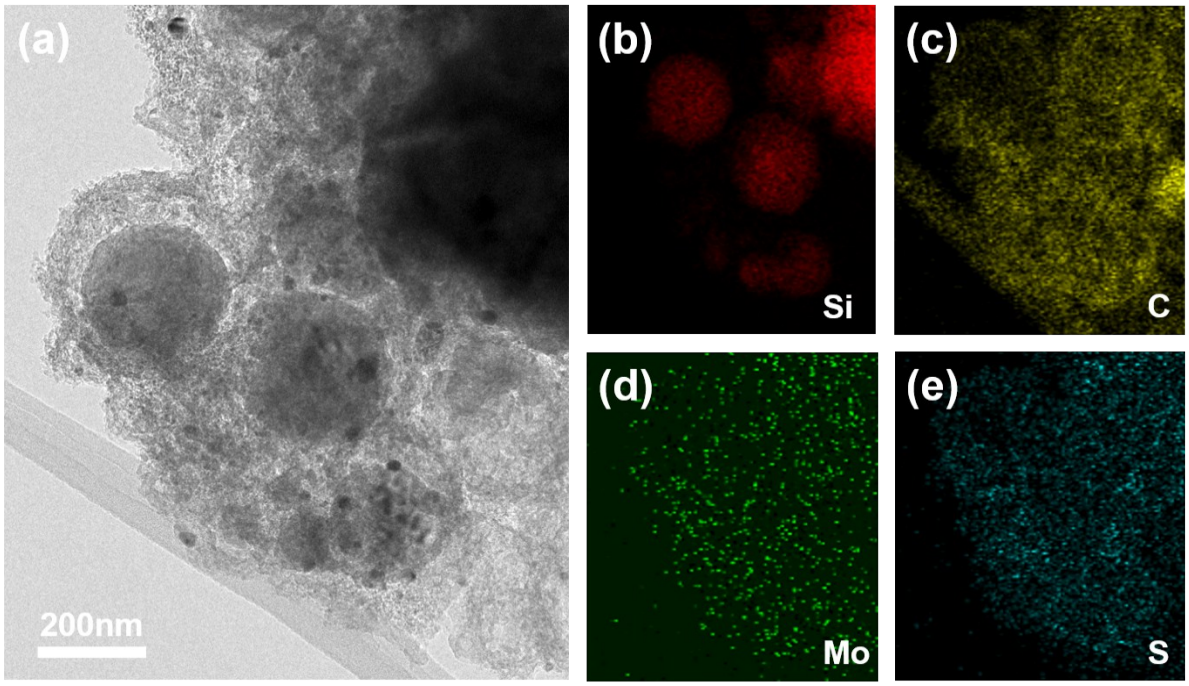

Figure S12. (a) TEM image of SCM1 electrodes after 100 cycles and its elemental mapping for (b) Si, (c) C, (d) Mo, and (e) S.

	Element (mass %)			
Composite	**Si**	**C**	**Mo**	**S**
Si@C	74.5	25.5	-	-
SCM1	36.5	9.1	32.6	21.8
SCM3	23.8	5.8	42.2	28.2
SCM5	10.5	3.2	51.8	34.5

Table S1. The composition of Si@C, SCM1, SCM3 and SCM5 obtained by X-ray fluorescence (XRF).

Shell thickness(nm)	Current density (mA/g)	Capacity retention (%)	Initial coulombic efficiency (%)	Capacity (mAh/g) (cycle number)	Rate performance (Capacity@Current density)	Reference
7	1^{st} : 400 $2^{nd} \sim 10^{th}$: 1200 $11^{th} \sim$: 4000	56	74	1583 (100)	1010mAh/g @8.4A/g	Nano Lett, 2012, 12, 3315-3321.
10	400	40	82	951 (100)	-	Adv. Funct. Mater, 2015, 25, 1426–1433.
10	50	29	71	610 (100)	860mAh/g @1Ag	Phys. Chem. Chem. Phys., 2015, 17, 17562-17565.
10.5	1^{st} : 100 2^{nd} : 200 $3^{rd} \sim$: 500	78	86	1451 (50)	428mAh/g @10A/g	This work (SCM1)
12	1^{st} : 100 $2^{nd} \sim 4^{th}$: 500 $5^{th} \sim$: 1000	35	74	780 (50)	250mAh/g @5A/g	Chem. Commun, 2014, 50, 5878-5880.
15.2	1^{st} : 100 2^{nd} : 200 $3^{rd} \sim$: 500	83	94	1205 (50)	558mAh/g @10A/g	This work (SCM3)
20 (inner:10, outer:10)	$1^{st} \sim 3^{rd}$: 100 $4^{th} \sim$: 500	71	-	1910 (50)	1009mAh/g @4A/g	J. Power Sources 2017, 342, 529-536.
27.5	1^{st} : 100 2^{nd} : 200 $3^{rd} \sim$: 500	92	97	754 (50)	695mAh/g @10A/g	This work (SCM5)
45	200	33	49	500 (50)	325mAh/g @2A/g	RSC adv, 2014, 4, 71-75.

Table S2. Comparison of the electrochemical properties of other Si@C yolk-shell structures.

Reference

[S1] A. R. Park, D. Y. Son, J. S. Kim, J. Y. Lee, N. G. Park, J. H. Park, J. K. Lee, P. J. Yoo, *ACS Appl. Mater. Interfaces*, 2015, **7**, 18483-18490.

[S2] X. Xiao, P. Lu, D. J. Ahn. *Adv. Mater*, 2011, **23**, 3911-3915.