Supporting Information

Improving Cycling Performance of Si-Based Lithium Ion Batteries Anode with Se-Loaded Carbon Coating

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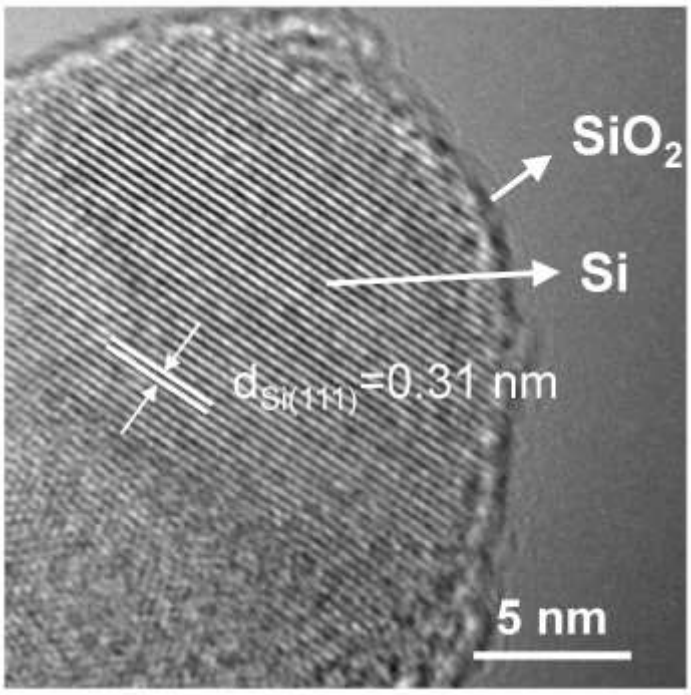

Figure S1. HRTEM image of Si@SiO_2 NP.

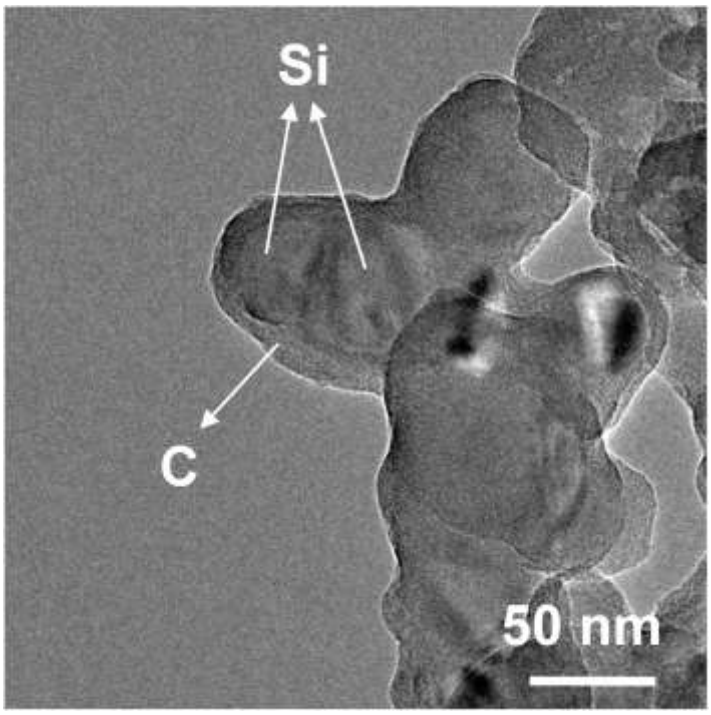

Figure S2. TEM image of Si@SiO_2@C/Se NPs.

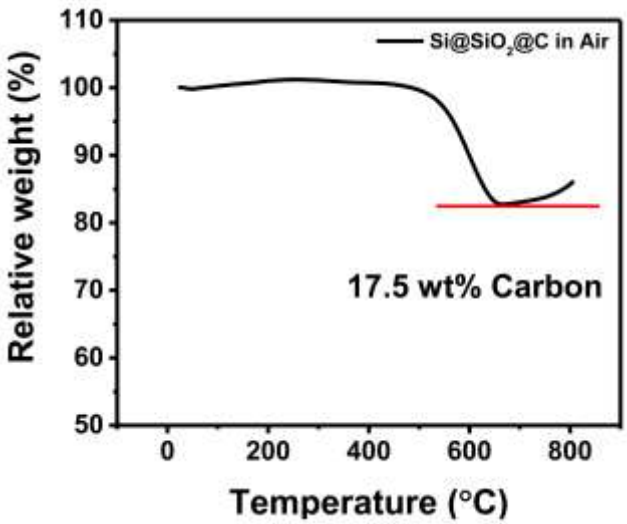

Figure S3. TGA curve of Si@SiO_2@C in Air.

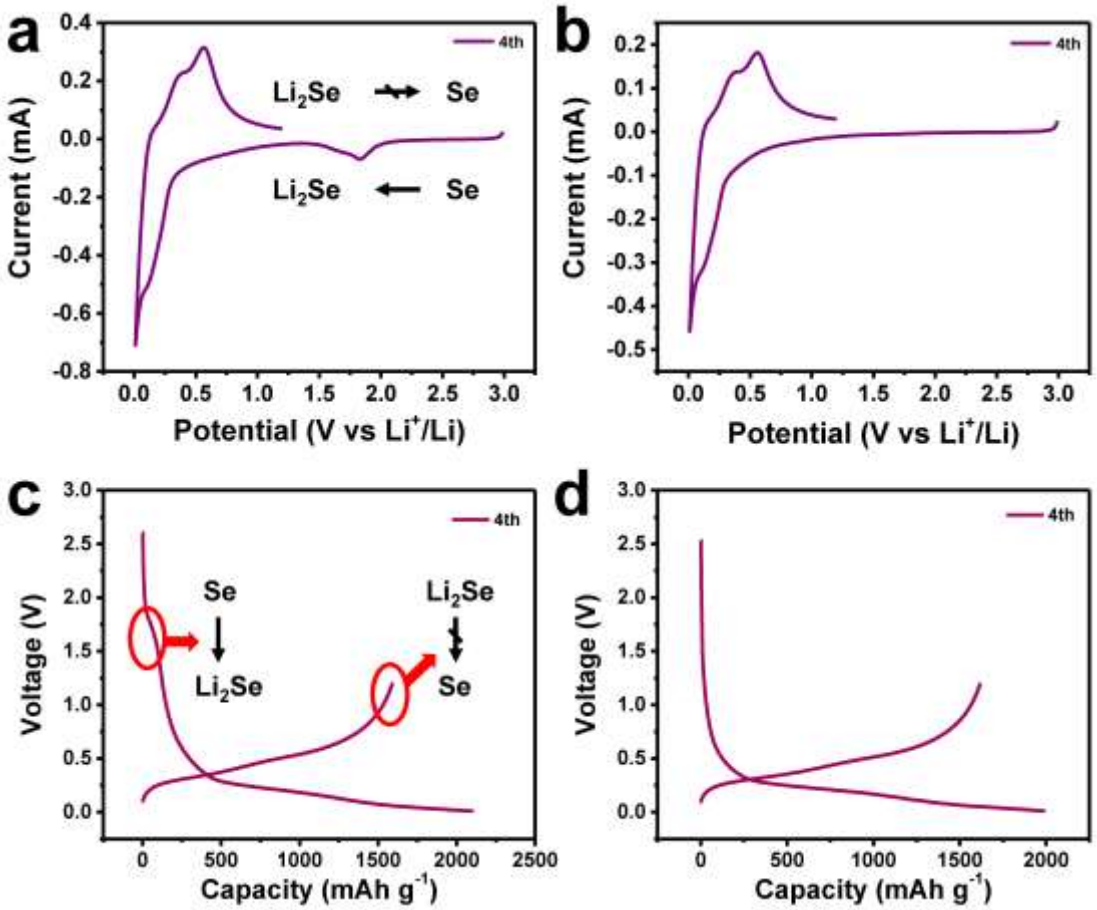

Figure S4. CV curves for (a) Si@SiO_2@C/Se and (b) Si@SiO_2@C electrode at a scan rate of 0.1 mV s^{-1} in the voltage range of 0.01-3 V and 0.01-1.2 V *vs* Li^+/Li; galvanostatic discharge/charge voltage profiles of the 4th cycle of (c) Si@SiO_2@C/Se and (d) Si@SiO_2@C electrode at 0.5 A g^{-1}.

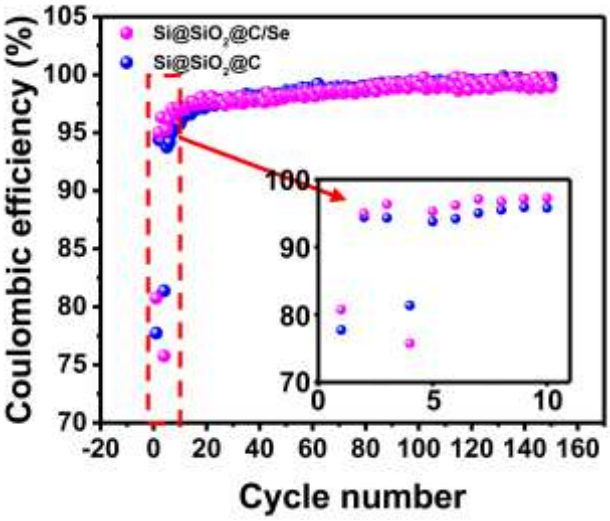

Figure S5. Coulombic efficiency of Si@SiO_2@C and Si@SiO_2@C/Se electrode in 150 cycles.

First-principles calculation

First-principles calculation is conducted using CASTEP.[1] generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) method is used to descript the exchange-correlation energy.[2] 310 eV energy cutoff and 2×2×1 k-point set with 0.01 eV/angstrom max force are used in geometric optimization.

Carbon framework is simulated by graphene layer since the interaction between graphite layers is negatable.[3] A double vacancy defect is used to simulate the micropores of carbon since it is one of the most common defects in graphene.[4] The bonding energy is calculated by the equation below: [5]

$$E_b = E_{C-Se} - (E_C + E_{Se})$$

Where E_b is bonding energy, E_{C-Se} is the total energy of graphene with Se bonded, E_C is the total energy of graphene and E_{Se} is the energy of Se. The calculated bonding energy between graphene and Se is 6.26 eV which indicates a strong bond

between Se and C atoms.

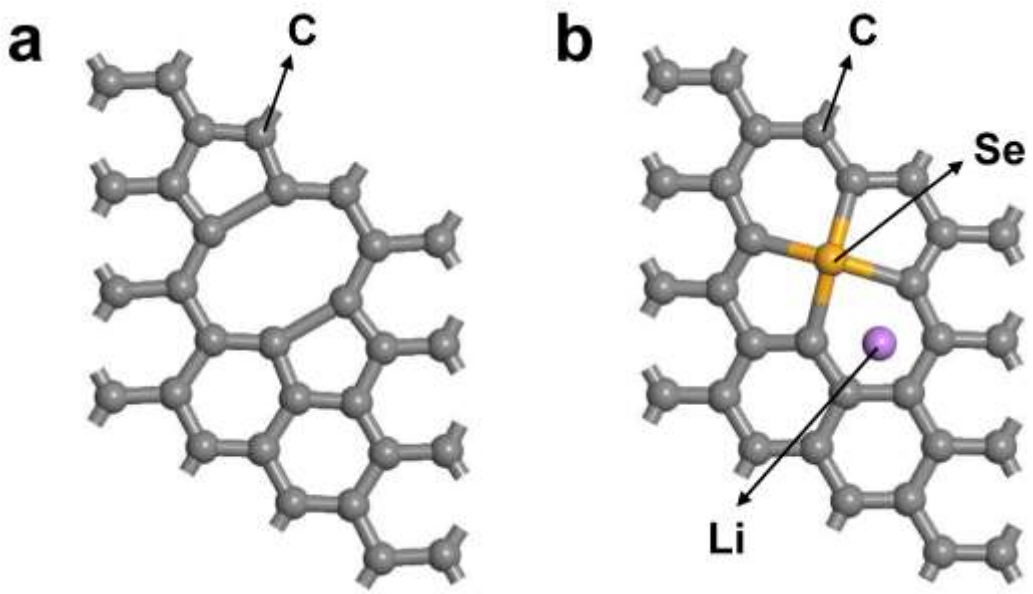

Figure S6. (a) Defect in carbon frame work and (b) Se loaded into carbon framework. The insertion of Se in Carbon defect leads to the bonding between Se and C with a strong bonding energy which enhances the structural stability of carbon film and SEI.

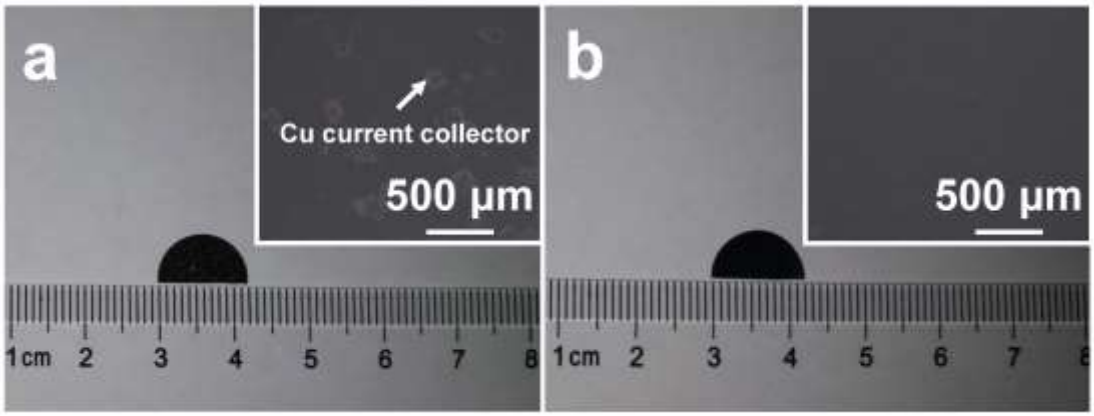

Figure S7. Photos and optical images of (a) Si@SiO_2@C and (b) Si@SiO_2@C/Se electrode after the 10th cycing.

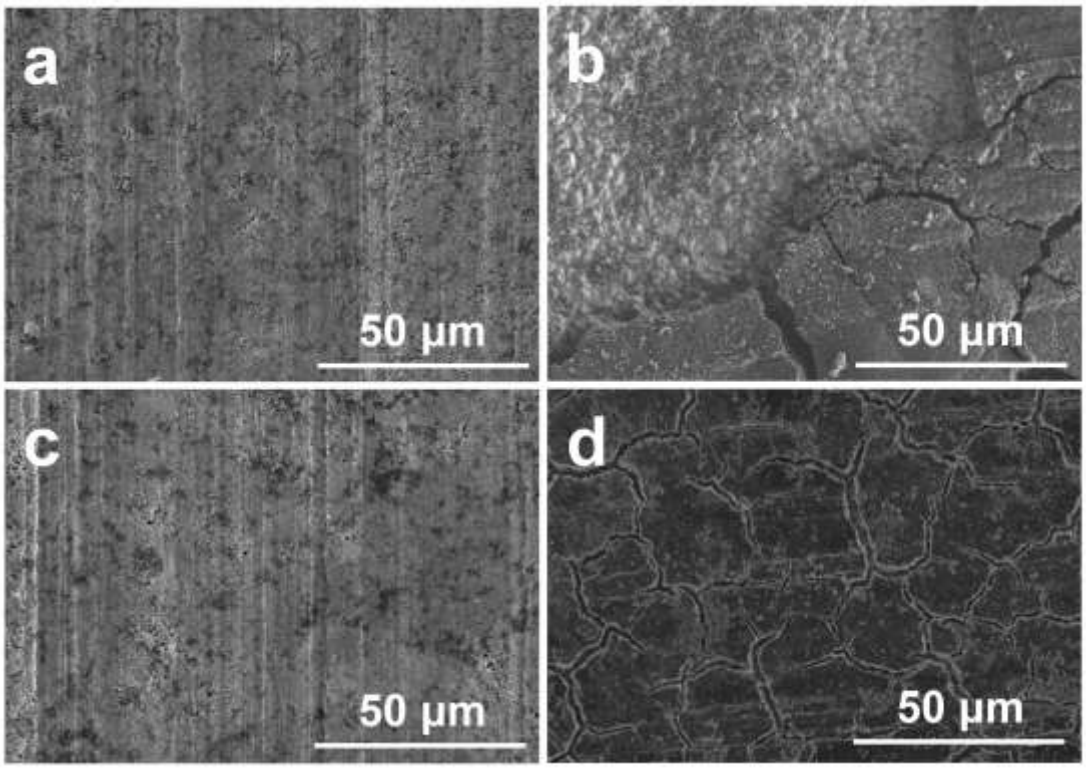

Figure S8. SEM images of Si@SiO_2@C and Si@SiO_2@C/Se electrodes before and after 10 cycling. (a), (c)Before cycling. (b), (d) after 10th cycling.

REFERENCE

1. Segall, M. D.; Lindan, P. J. D.; Probert, M. J.; Pickard, C. J.; Hasnip, P. J.; Clark, S. J.; Payne, M. C., First-principles simulation: ideas, illustrations and the CASTEP code. *Journal of Physics-Condensed Matter* **2002**, 14, 2717-2744.
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3. El-Barbary, A. A.; Telling, R. H.; Ewels, C. P.; Heggie, M. I.; Briddon, P. R., Structure and energetics of the vacancy in graphite. *Phys. Rev. B* **2003**, 68, 144107.
4. Zhou, L. J.; Hou, Z. F.; Wu, L. M., First-Principles Study of Lithium Adsorption and Diffusion on Graphene with Point Defects. *J. Phys. Chem. C* **2012**, 116, 21780-21787.
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