

Electronic Supplementary Information

Bamboo Leaves Derived Ultrafine Si Nanoparticles and Si/C Nanocomposites for High-performance Li-ion Battery Anodes

Lei Wang ^a, Biao Gao ^b, Changjian Peng ^a, Xiang Peng ^c, Jijiang Fu ^b, Paul K Chu ^c and Kaifu Huo ^{a*}

^a *Wuhan National Laboratory for Optoelectronics(WNLO), Huazhong University of Science and Technology, Wuhan 430074, China.*

^b *The State Key Lab for Refractory and Metallurgy, Wuhan University of Science and Technology, Wuhan 430081, China*

^c *Department of Materials Science and Physics, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong, China*

[*] E-mail: kfhuo@hust.edu.cn



Figure S1. Optical photograph of HC-leached dead bamboo leaves (BLs).

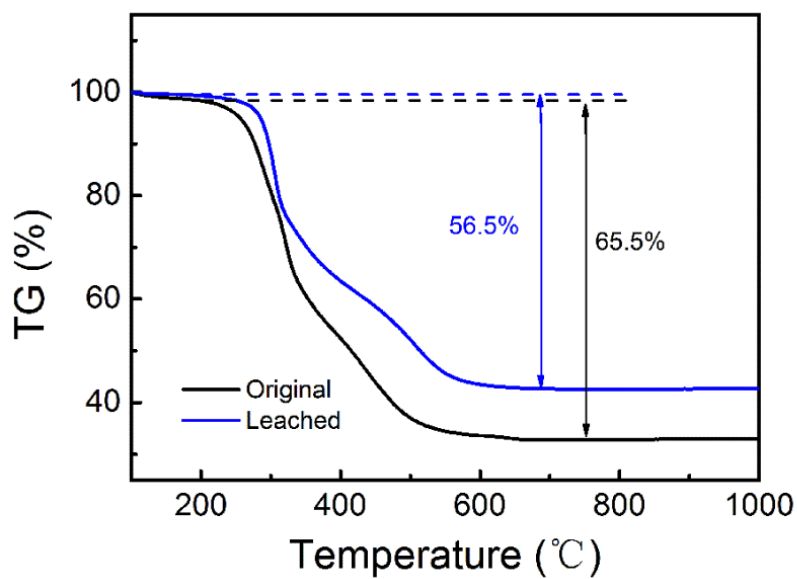


Figure S2. TG Curves for original BLs and HCl-leached BLs, suggesting the carbon weighs about 56.5% of HCl-leached BLs.

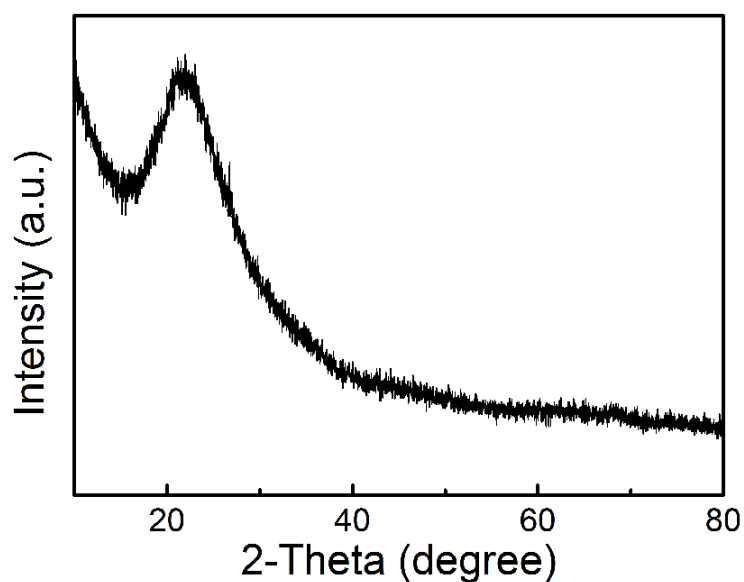


Figure S3. XRD pattern for SiO₂. A broad peak at around 22.5° indicates the amorphous characteristic of silica derived from BLs

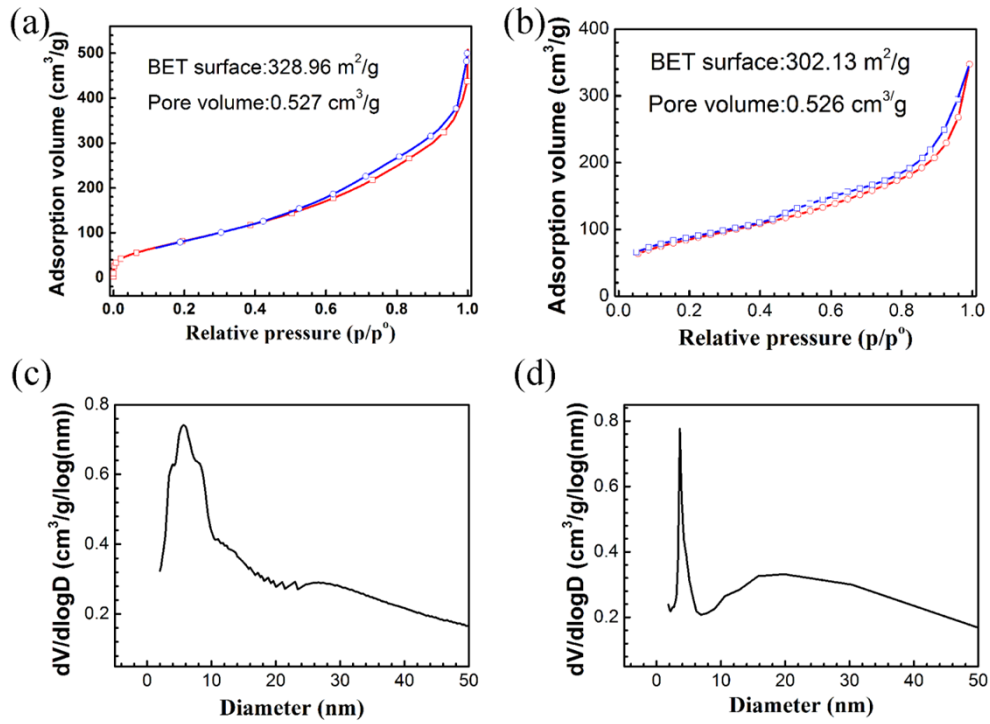


Figure S4. BET results for silica and silicon. (a-b) Isothermal of BLs derived SiO₂ and Si NPs. (c-d) pore distribution for BLs derived SiO₂ and Si NPs.

Assuming that the silicon NPs are absolute spherical particles with radius r and density ρ .

The mass :

$$m = \rho V = \rho \frac{4\pi r^3}{3}$$

The surface area : $S = 4\pi r^2$

The surface area could be calculated:

$$S_{bet} = \frac{S}{m} = \frac{4\pi r^2}{\frac{4\pi r^3}{\rho \frac{3}{r}}} = \frac{3}{\rho r}$$

Since the density of crystalline silicon is 2.33 g cm⁻³ and testing results showed the BET surface is 302 m²/g, thus, the radius is calculated:

$$r = \frac{3}{\rho S_{bet}} = 4.2 \text{ (nm)}$$

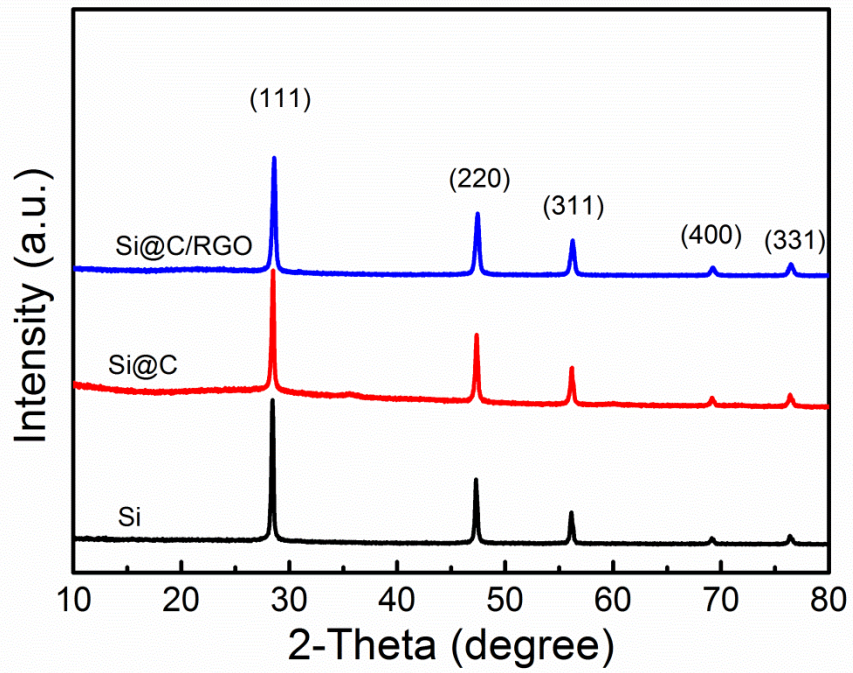


Figure S5. XRD patterns for Si, Si@C and Si@C/RGO, suggesting that the Si in Si@C and Si@C/RGO composite remain crystalline structure.

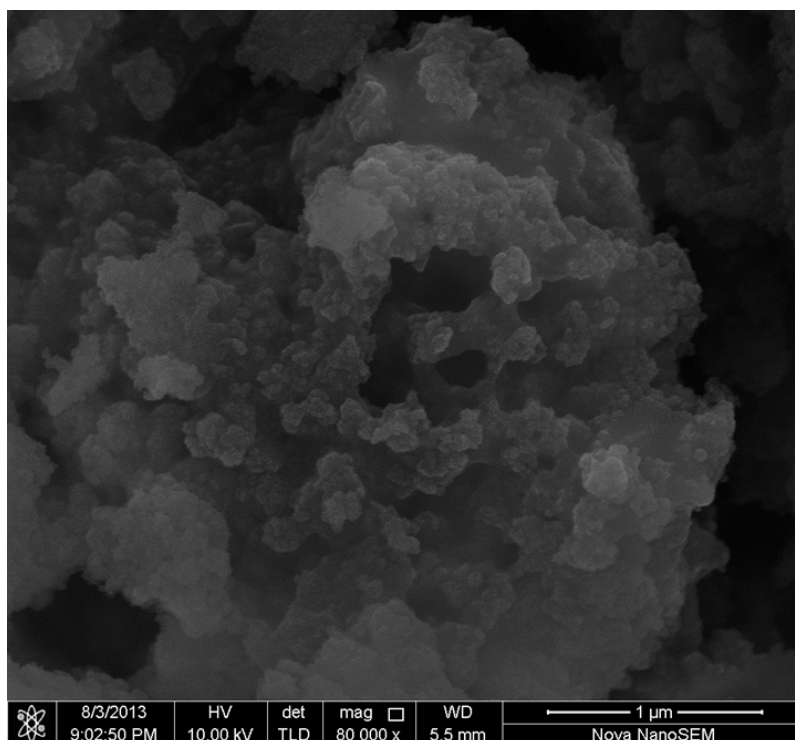


Figure S6. BLs derived Si produced by magnesiothermic reduction of BLs derived SiO₂ without adding NaCl as the heat-scavenger. Only large Si particles sintered together with a size of ten micrometers are prepared due to the large heat release from the highly exothermic reaction. The high local temperature (over 1720 °C) can collapse the architecture of the nanosized SiO₂ precursor and fuse and agglomerate the as-synthesized Si into large crystals, resulting in the formation of bulk Si.

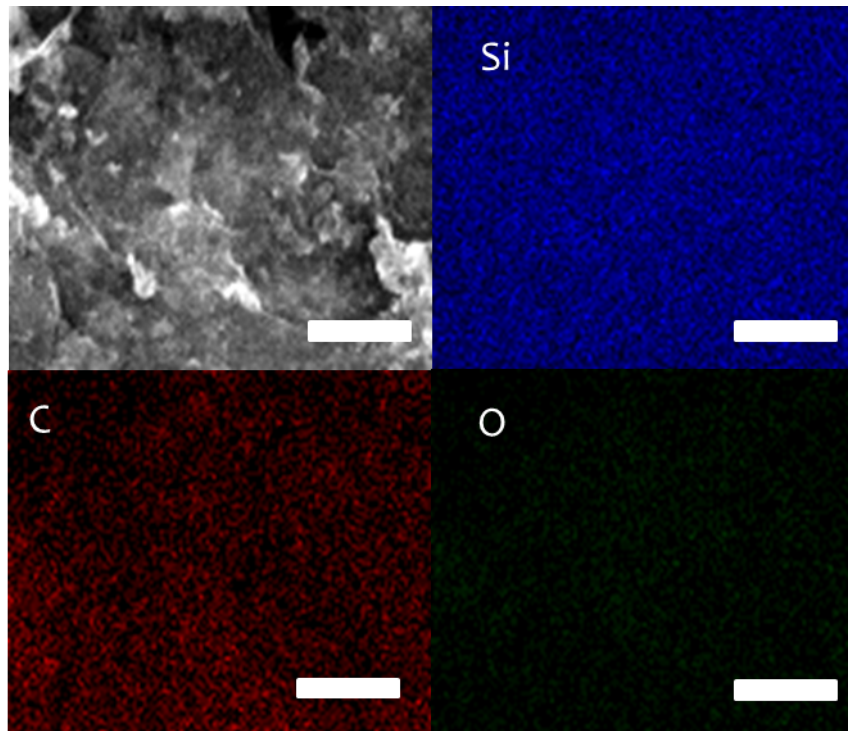


Figure S7. EDS Mapping for the sample of Si@C/RGO nanocomposites. The scale bar is 30 μm . The C and Si are well dispersed in the whole image, indicating the Si were well dispersed in Si@C/RGO nanocomposites

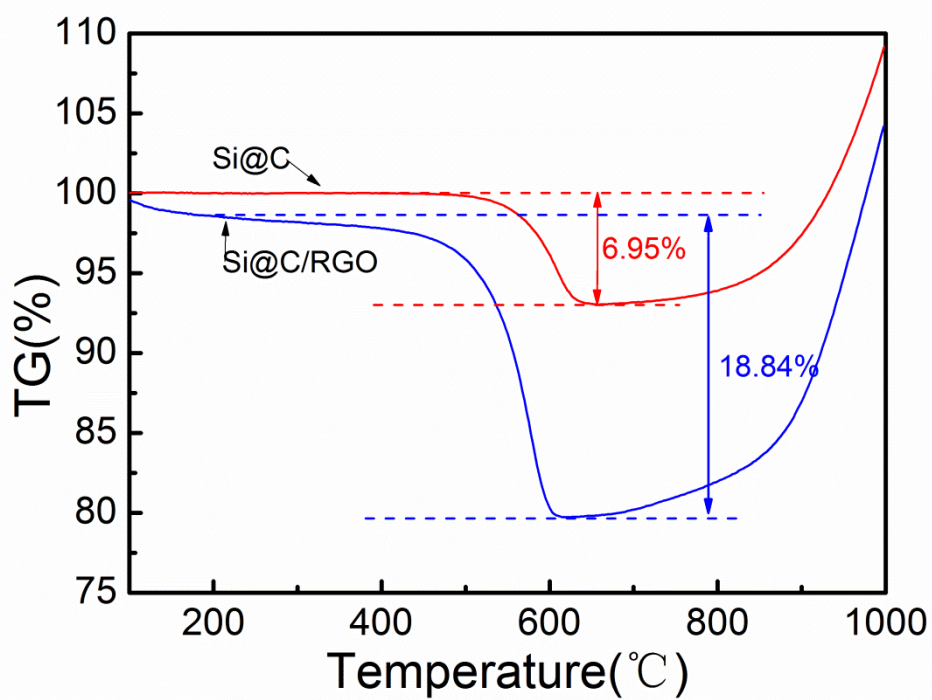


Figure S8. TG curves for Si@C and Si@C/RGO, indicate that the C coating and RGO contribute about 6.9% and 11.9%, respectively, and so the weight of Si in Si@C/RGO nanocomposites is 82.2%

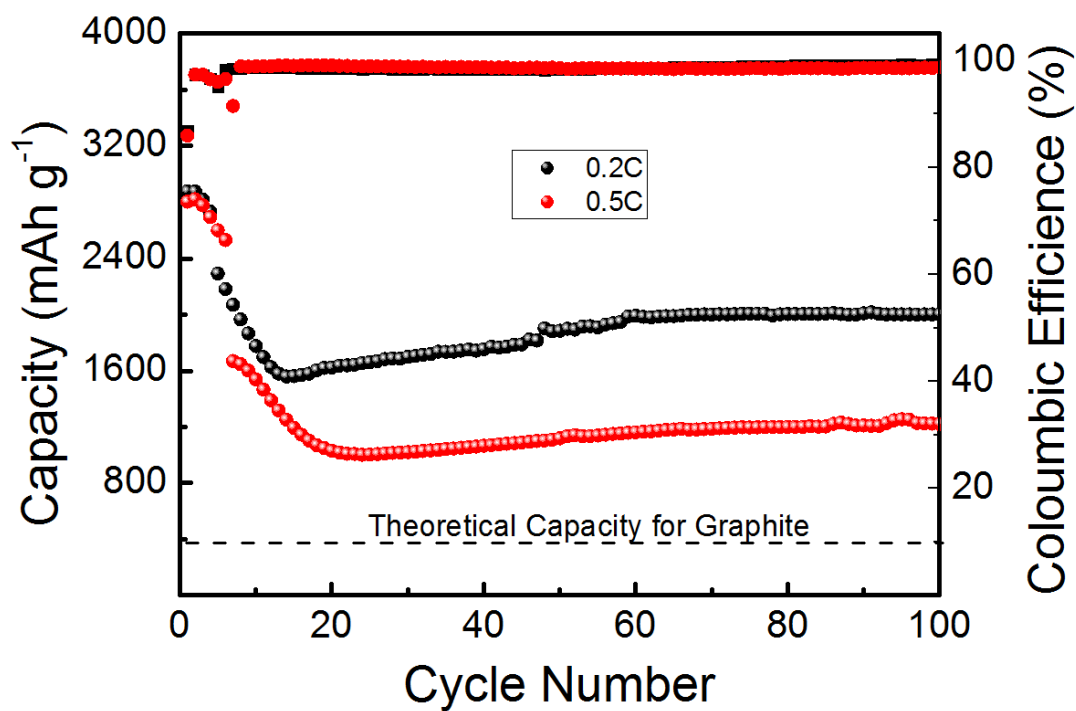


Figure S9. Discharging capacity curves of the Si NPs versus cycle number at 0.2C and 0.5C rates. The BLs-derived Si NPs exhibit good cycle stability and high specific capacity of 1,800 and 1,200 mAh/g at 0.2 C and 0.5 C rates after 100 cycles, which are 4.8 and 3.2 times larger than the theoretical capacity of graphite.

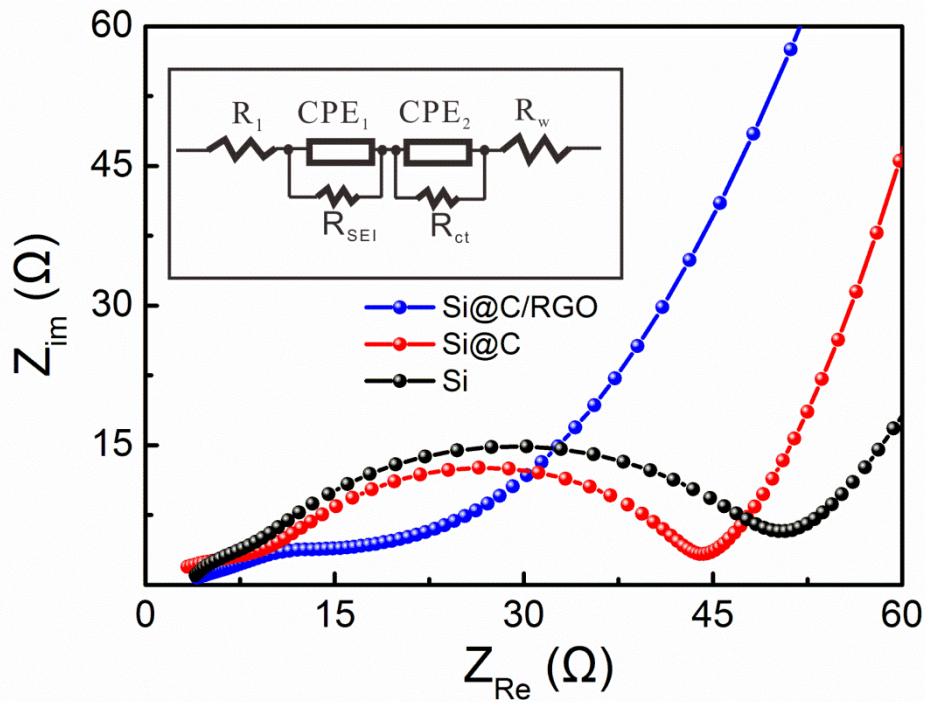


Figure S10. The Nyquist plots the equivalent circuit for the Si, Si@C and Si@C/RGO electrodes.

In the equivalent circuit, R_1 is composed of electrolyte resistance (R_s) and electrode resistance (R_e); R_{SEI} represents the SEI resistance; R_{ct} represents the charge-transfer resistance across the electrode-electrolyte interface; CPE_1 is the constant-phase element which represents the diffusion capacitance attributed to Li-ion diffusion in SEI film and CPE_2 is the electric double-layer capacitance of electrode-solution interface. The Warburg element represents impedance due to diffusion of ions into the active material of the electrode

The Capacity contributed by the Carbonaceous Components:

The capacity contributions from carbonized PDA, Carbon Black and RGO were calculated on the following procedure:

Capacity contribution of carbon black in Si@C electrode(%):

Weight content of carbon black \times Capacity of carbon black / Capacity of Si@C electrode = $0.2 \times 170 / 1850 \times 100\% = 1.8\%$

Capacity contribution of carbonized PDA in Si@C electrode(%):

Weight content of carbonized PDA \times Capacity of carbonized PDA / (Capacity of Si@C electrode - Weight content of carbon black \times Capacity of carbon black) = $0.069 \times 196 / (1850 - 0.018 \times 170) \times 100\% = 0.7\%$

Capacity contribution of RGO in Si@C/RGO electrode(%):

Weight content of RGO \times Capacity of RGO / (Capacity of Si@C/RGO electrode - Weight content of carbon black \times Capacity of carbon black) = $0.119 \times 524 / (1900 - 0.018 \times 170) \times 100\% = 3.28\%$

Capacity contribution of carbonized PDA in Si@C/RGO electrode(%):

Weight content of carbonized PDA \times Capacity of carbonized PDA / (Capacity of Si@C/RGO electrode - Weight content of carbon black \times Capacity of carbon black) = $0.069 \times 196 / (1900 - 0.018 \times 170) \times 100\% = 0.7\%$

*The capacity of carbon black and carbonized PDA is based on *Proc. Natl. Acad. Sci. U. S. A.*, 2013, **110**, 12229-12234

*The capacity of RGO is based on *Electrochem. Commun.*, 2011, **13**, 1332-1335.