[Electronic Supplementary Information]

Titanium Nitride Coating to Enhance the Performance of Silicon Nanoparticles as a Lithium-Ion Battery Anode

Duihai Tang, Ran Yi, Mikhail L. Gordin, Michael Melnyk, Fang Dai, Shuru Chen, Jiangxuan Song and Donghai Wang*

Department of Mechanical and Nuclear Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802, United States.

* To whom correspondence should be addressed. Tel: +1 814 863 1287

E-mail: dwang@psu.edu

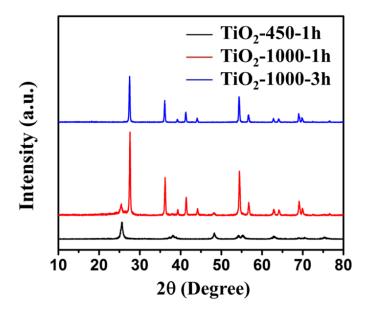


Fig. S1. XRD patterns of TiO_2 -450-1h, TiO_2 -1000-1h, and TiO_2 -1000-3h.

To demonstrate that the silicon can act as the catalyst, we synthesized the TiO₂ through the same procedure of Si@TiO₂, but without the addition of silicon. This TiO₂ was thermally annealed in a in a tube furnace at 450 °C for 1 h under nitrogen stream, this material was named TiO₂-450-1h. And then TiO₂-450-1h was annealed at 1000 °C for 1h and 3 h, respectively under nitrogen stream, these two samples were named TiO₂-1000-1h and TiO₂-1000-3h, respectively. As shown in Figure 1S, all the peaks of TiO₂-450-1h can be assigned to the anatase phases and all the peaks of TiO₂-1000-3h can be assigned to the rutile phases. We can draw a conclusion that, the TiO₂ could not react with N₂ to form the TiN without the silicon at 1000 °C. The overall reaction to form TiN at 1000 °C is denoted in the following equations:^{S1}

$$3Si + 2N_2 = Si_3N_4, (1)$$

$$Si_3N_4 + TiO_2 = TiN + N_2O + NO + 3Si.$$
 (2)

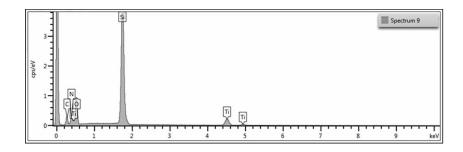


Fig. S2. EDS spectrum of Si@TiN.

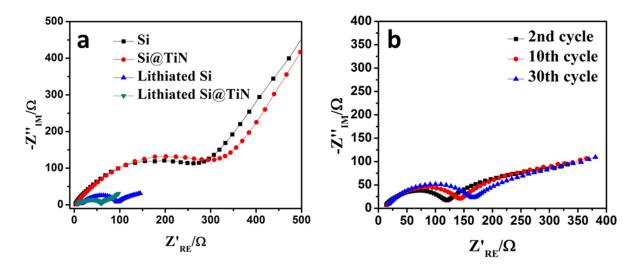


Fig. S3. (a) Nyquist plots of Li-ion cells using Si and Si@TiN electrodes at open circuit potential of approximately 2.90 V (vs. Li⁺/Li) and using lithiated Si and lithiated Si@TiN electrodes after the initial discharge to the potential of approximately 0.05 V (vs. Li⁺/Li). (b) Nyquist plots of Li-ion cells using Si@TiO₂ electrodes for cycles at 2nd, 10th and 30th.

References

S1 Yu. F. Kargin, S. N. Ivicheva, A. S. Lysenkov, N. A. Ovsyannikov, L. I. Shvorneva and K. A. Solntsev, *Inorg. Mater.* 2012, **48**, 897-902.