[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 TiO$_2$ through the same procedure of Si@TiO$_2$, but without the addition of silicon. This TiO$_2$ was thermally annealed in a tube furnace at 450 °C for 1 h under nitrogen stream, this material was named TiO$_2$-450-1h. And then TiO$_2$-450-1h was annealed at 1000 °C for 1 h and 3 h, respectively under nitrogen stream, these two samples were named TiO$_2$-1000-1h and TiO$_2$-1000-3h, respectively. As shown in Figure 1S, all the peaks of TiO$_2$-450-1h can be assigned to the anatase phases and all the peaks of TiO$_2$-1000-3h can be assigned to the rutile phases. We can draw a conclusion that, the TiO$_2$ could not react with N$_2$ 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:

\[
3\text{Si} + 2\text{N}_2 = \text{Si}_3\text{N}_4, \quad (1)
\]

\[
\text{Si}_3\text{N}_4 + \text{TiO}_2 = \text{TiN} + \text{N}_2\text{O} + \text{NO} + 3\text{Si}. \quad (2)
\]
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