Supporting Information

Nitrogen-Doped Graphitic Layers Deposited on Silicon Nanowires for Efficient Lithium-Ion Battery Anodes

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Figure S1. Survey scanned XPS of the Si NWs and Si-CNₓ NCs, measured using photon energy of 630 eV. The N 1s peak intensity increases with increasing N content.
**Figure S2.** (a) HRTEM image of the Si NW sample (mixed with carbon black binder and PVDF) after Li extraction at 45 cycles. Most of crystalline Si NWs crack into amorphous or crystalline phase NPs. HRTEM images of the (b) SC1 and (c) SCN1, showing that the NCs degraded not much after 45 cycles. (d) Their Si NW core partially break into the amorphous or crystalline NPs (size $\leq$ 5 nm) embedded in the crystalline graphitic layers. The graphitic layers remain with the (002) planes separated by a distance of 3.4 Å. The FFT image shows a ring pattern, indexed as $\text{Li}_{12}\text{Si}_7$ and/or $\text{Li}_{22}\text{Si}_5$ phase (top inset). The $d$ spacing of crystalline NPs is 2.1 Å, which is close to (281) planes of $\text{Li}_{12}\text{Si}_7$ (JCPDS No. 40-0942; orthorhombic $a = 8.600$ Å; $b = 19.75$ Å; $c = 14.336$ Å) and/or (048) planes of $\text{Li}_{22}\text{Si}_5$ (JCPDS No. 40-0942; cubic $a = 18.75$ Å), as shown in the bottom inset.
**Figure S3.** The most stable configuration for 9 (a), 12 (b) and 16 (c) Li-intercalated SYSTEM N. Four supercells are shown in which each supercell consists of $4 \times 4$ graphene sheet. One Li atom is not visible for 12 Li-intercalation case, because it is located below one of C atoms of the upper graphene sheet.
**Figure S4.** The most stable configuration for 9 (a), 12 (b) and 16 (c) Li-intercalated SYSTEM H. Four supercells are shown in which each supercell consists of $4 \times 4$ graphene sheet. For clarity, the upper graphene sheet is represented by ball-and-stick model, while the lower sheet is shown in stick model. In Figure 4, only one supercell is shown for 16 Li-intercalated system.
Figure S5. The most stable configuration for 9 (a), 12 (b) and 16 (c) Li-intercalated SYSTEM C. One N atom in the lower graphene sheet is not visible. One Li atom is not visible for 9 Li-intercalated case, since it is located below one of C atoms of the upper graphene sheet. Four supercells are shown in which each supercell consists of $4 \times 4$ graphene sheet.