Supporting Information for

Penta-SiCN monolayer as a well-balanced performance anode material for Li-ion batteries

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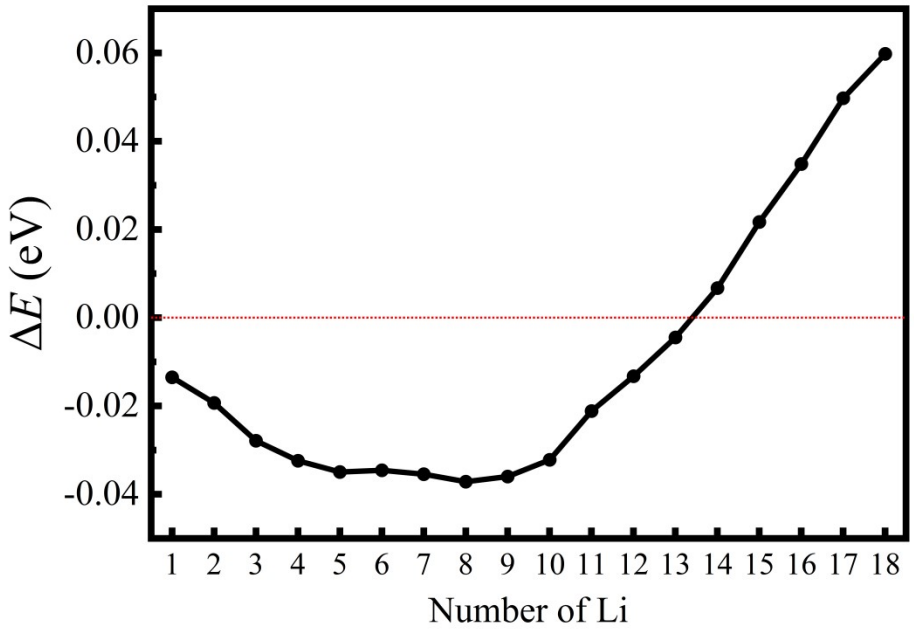

Fig. S1. The energy difference ($\Delta E = E_{S1} - E_{S3}$) between two configurations. The E_{S1} and E_{S3} represents the total energy of two configurations with Li adsorbed on S1 and S3 sites of penta-SiCN monolayer, respectively.

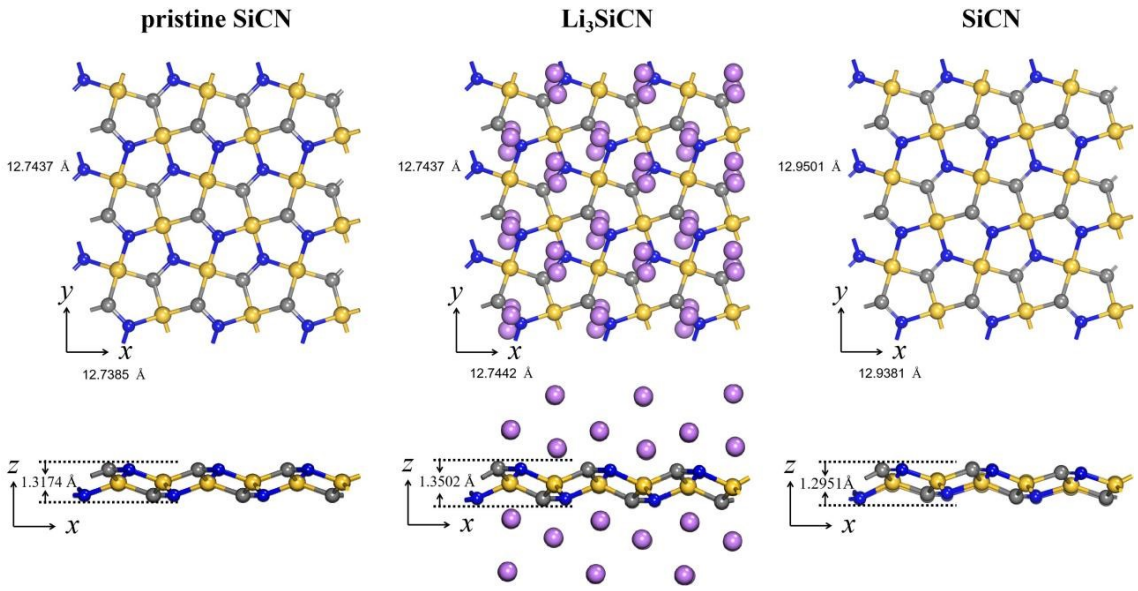

Fig. S2. The optimized configuration of (a) pristine penta-SiCN, (b) penta-SiCN with multi-layers adsorption of Li (Li_3SiCN), and (c) penta-SiCN after complete removal of Li atoms at the maximal concentration of Li adsorption (Li_3SiCN).