Supporting Information

Adsorption of Li on Sing-Layer Silicene for Anodes of Li-ion Batteries

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Figure S1

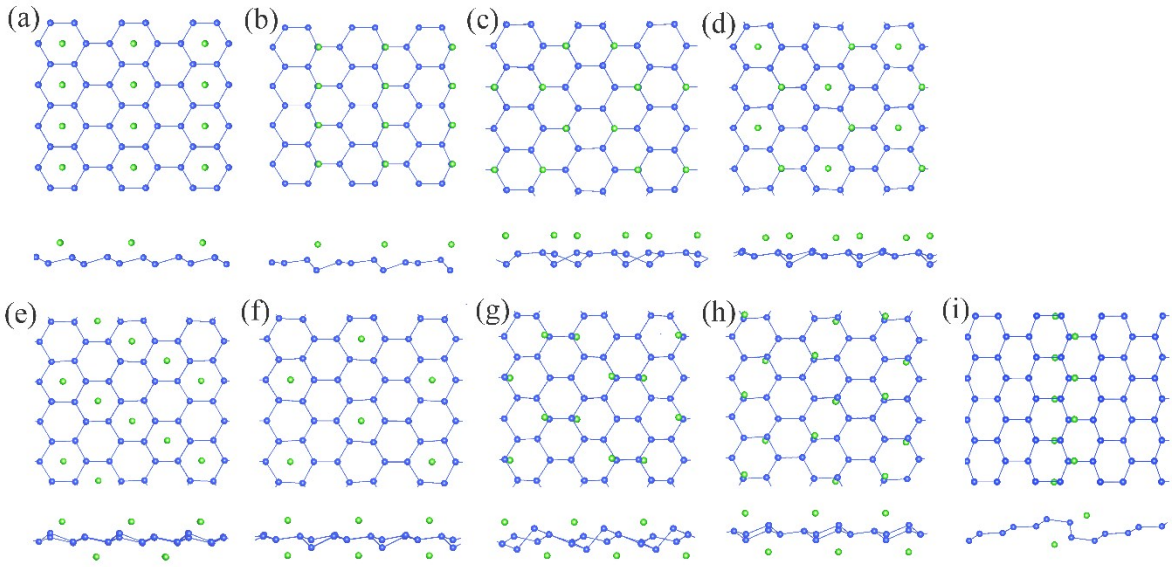

Figure S1. The top and side views of atomic structures of the models for Li adsorption on silicene with x=0.5, including the adsorption on (a) hollow site with upper surface, on (b)-(c) top site with upper surface, (d) the mixing model with top and hollow sites of upper

surface, (e)-(f) on hollow sites with up-down surfaces, and (g)-(i) on top sites with un-down surfaces. It is noticed the model of Li up-down chains (i) is the most stable among the models (g-i) about top sites with up-down surfaces.

Table S1

The adsorption energies of the models in Figure S1 for x=0.5. Among these models, the model of up-down chains is the most stable.

No.	E_{ad} (eV/Li)	Category
a	-2.011	hollow site with upper surface
b	-1.890	top site with upper surface
c	-1.915	
d	-2.024	mixing model with top and hollow
e	-2.080	hollow sites with up-down surfaces
f	-2.110	
g	-2.141	hollow sites with up-down surfaces
h	-1.937	
i	-2.326	

Figure S2

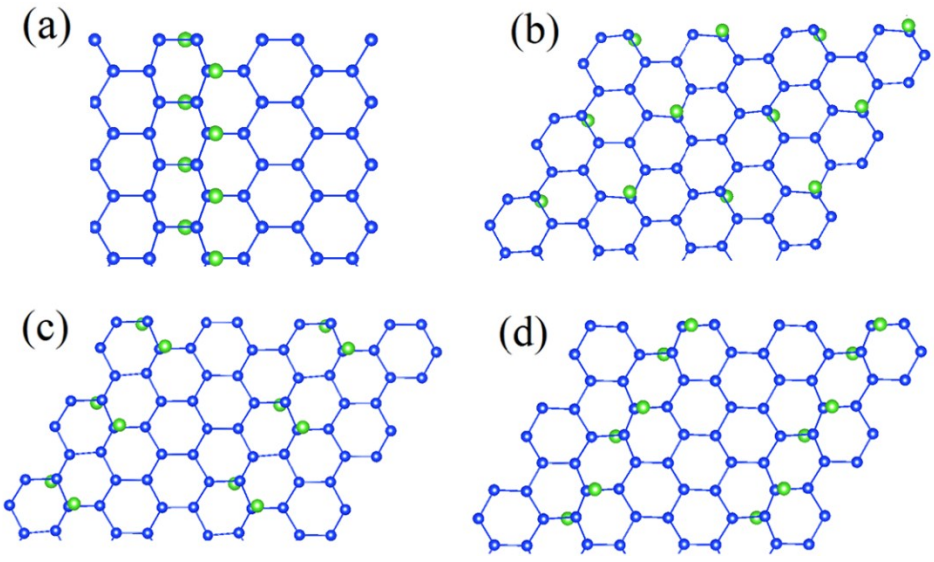

Figure S2. The top and side views of atomic structures of the models for Li adsorption on

silicene with x=0.167, including (a) the adsorption on top with up-down chain, (b) isolated up-adsorption and down-adsorption on top sites, (c-d) adsorption on top with isolated up-down pairs, in order to checking the relative stability of the up-down chain model in Figure S2. The adsorption energies of four models (a, b, c and d) are -2.263 eV/Li, -2.046 eV/Li, -1.979 eV/Li, and -1.901 eV/Li, respectively.

Figure S3

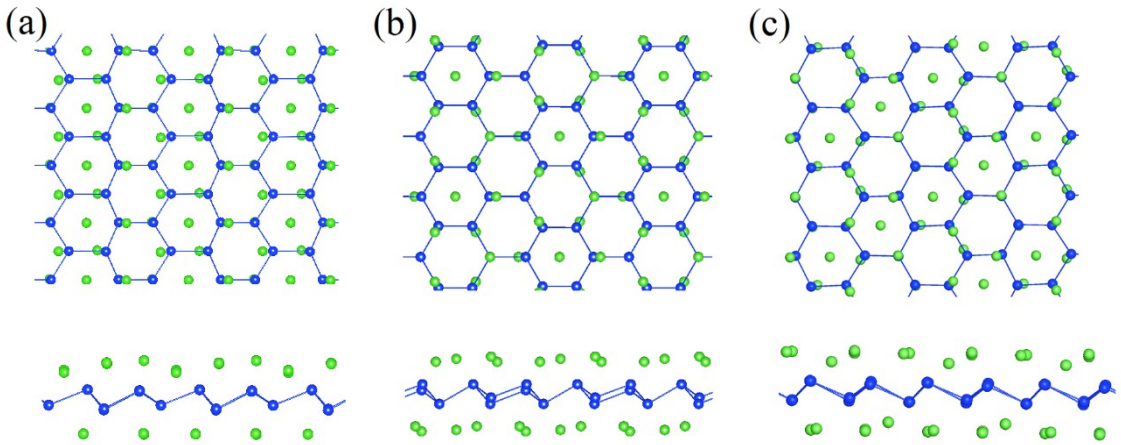

Figure S3. The top and side views of atomic structures of the models for Li adsorption on LiSi with *x*=1.25, including (a) the adsorption on hollow of upper surface, model-1, (b) on both surfaces with up-down pair, model-2, (c) on both surfaces with up-down chain along zigzag direction, model-3, in order to checking the breaking of Si-Si bonds by comparing with the model-4 in Figure 1f. The adsorption energies of model-1, 2 and 3 are -2.066 eV/Li, -2.064 eV/Li, and -2.054 eV/Li, respectively.

Figure S4

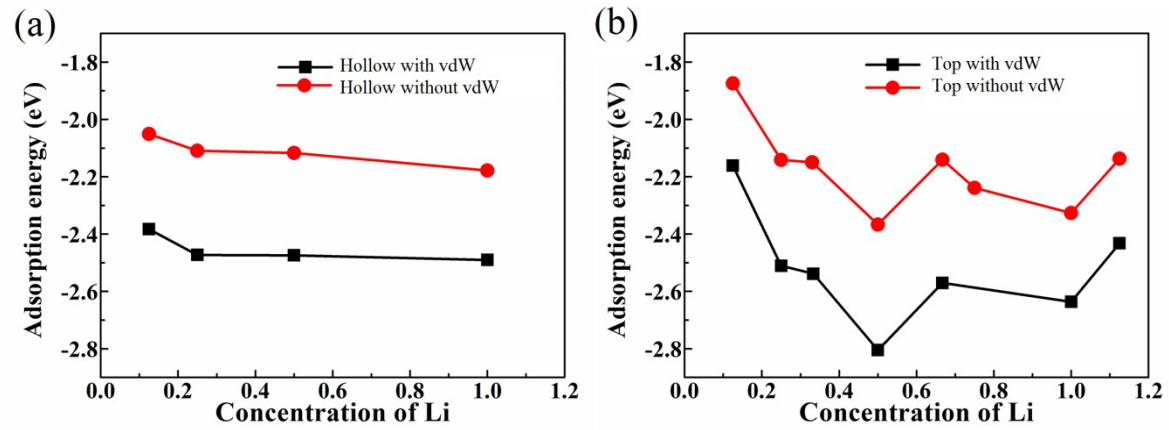

Figure S4. The analysis of van der Walls effect with the change of Li concentration for Li adsorption on (a) hollow site and (b) top site. It is found that there is no obvious change for the contribution of van der Walls, following the increase of Li concentration.

Figure S5

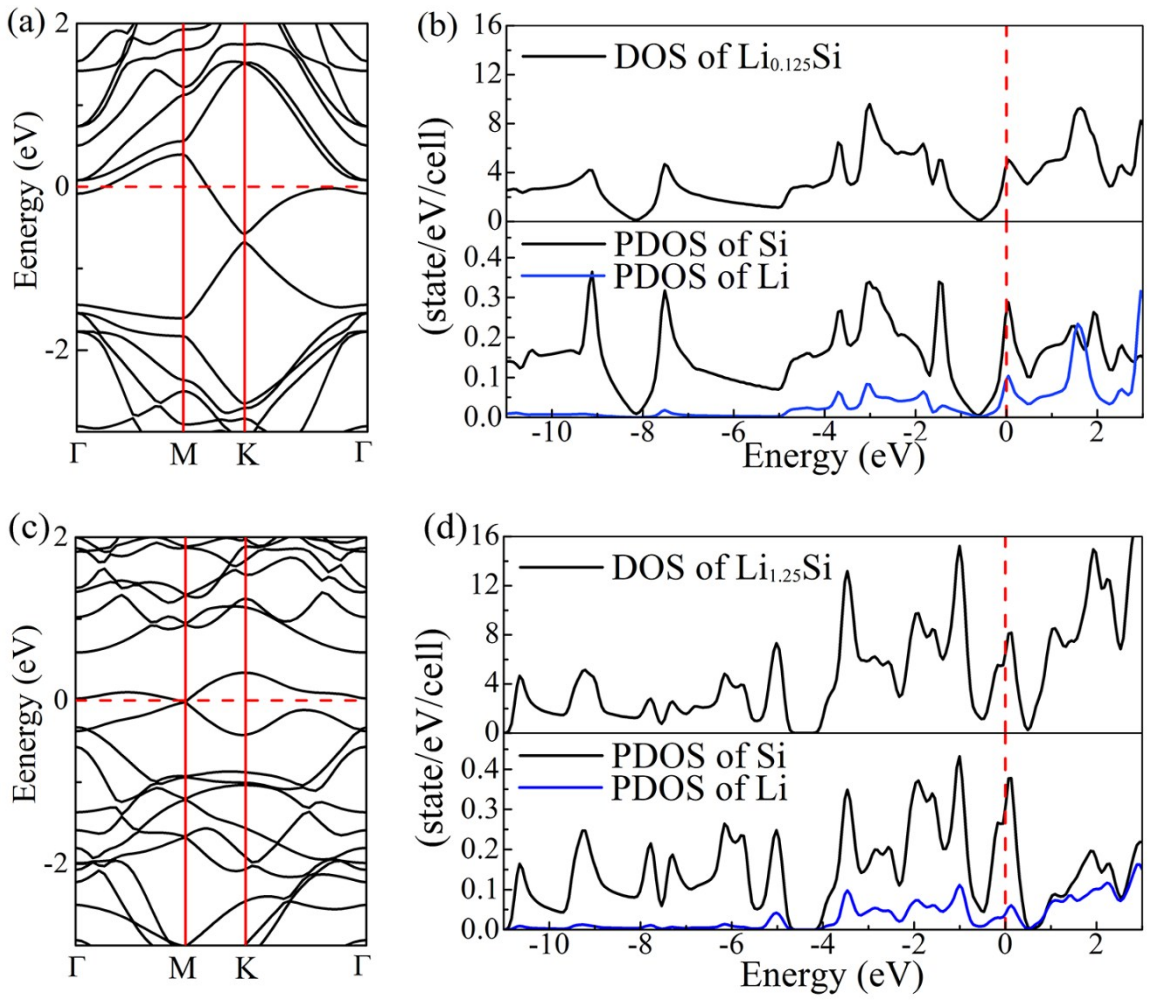

Figure S5. The band structures, density of states (DOS) and the partial density of states (PDOS) of (a, b) the model of Li adsorption on hollow site with x=0.125, and (c, d) the model of Si-Si breaking with x=1.25 in Figure 1f.

Figure S6

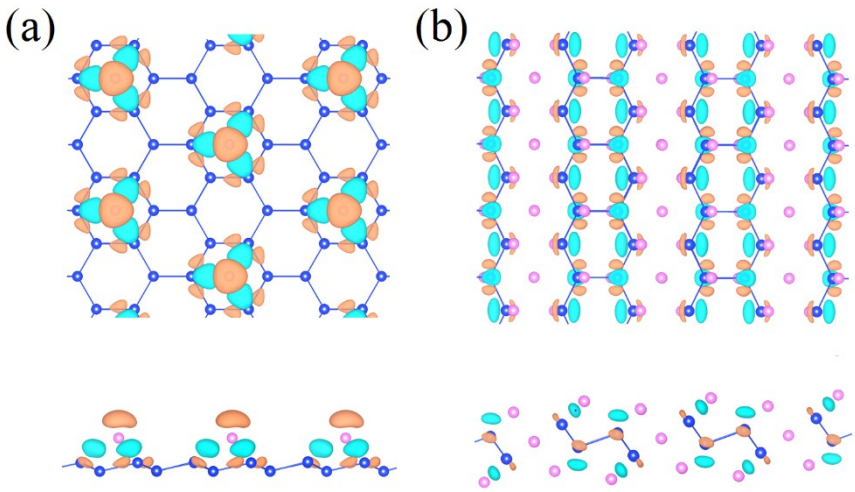

Figure S6. The top and side views of charge-density redistributions for (a) the model of Li adsorption on hollow site with x=0.125, and (b) the model of Si-Si breaking with x=1.25 in Figure 1f.

Figure S7

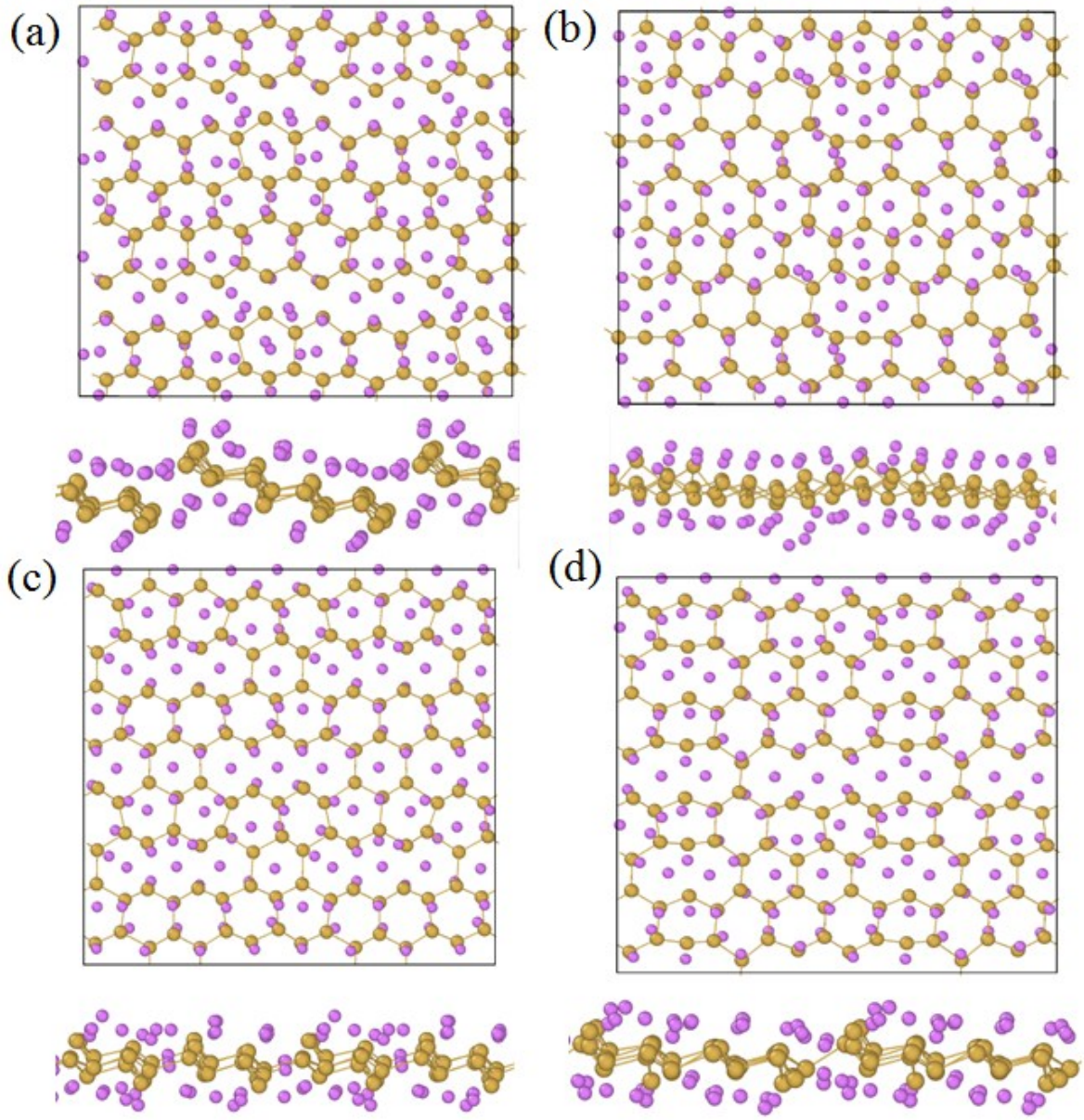

Figure S7. Snapshots of structures about $Li_{1.25}Si$ in MD processes for model-1 at temperature 300 K (a) and 500K (b) in Figure S3a of SI and model-4 at 300 K (c) and 500 K (d) in Figure 1f.