Supplementary material:

Strain or electric field induced direct bandgap in ultrathin silicon film and its application as photovoltaics or photocatalyst

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Multilayer silicene (MLS) can adopt different stacking patterns. Among them, ABA... and ABC… stacking configurations are relative stable. Experimental observations (Wu et al (DOI: 10.1038/srep13590) also demonstrate MLS films (MLS-F) mainly adopt the ABC stacking patterns. Based on these researches, we provide MLS structural models in Figure S1. The results demonstrate that MLSs automatically evolve into ultrathin silicon films with induced surface dangling bonds. Because of these surface states, MLS-Fs exhibit metallic characters (Figure S1 (f, g)).

In order to make our structural more clear and compare silicon films in different orientations, the (111), (110) and (100) silicon films got from the diamond bulk silicon are also provided in Figure S2. (111) silicon films exhibit hexagonal structures and the C3 symmetry (Figure S2 (a)). (110) silicon films have the rectangular structure and C2 symmetry (Figure S2 (b)). (100) films adopt tetragonal structure with C4 symmetry (Figure S2 (c)). Moreover, it can be observed from Figure S1 and Figure S2 that MLS-F in ABC stacking are just the silicon film in the (111) direction.

Figure S3 provides the total energy of ultrathin hydrogenated silicon films (USF), under zero in-plane strain. The results demonstrate that the increase in the number of silicon layers gradually reduces the total energy of these structures. Hence, the formation of these multilayer USFs is energy favorable.

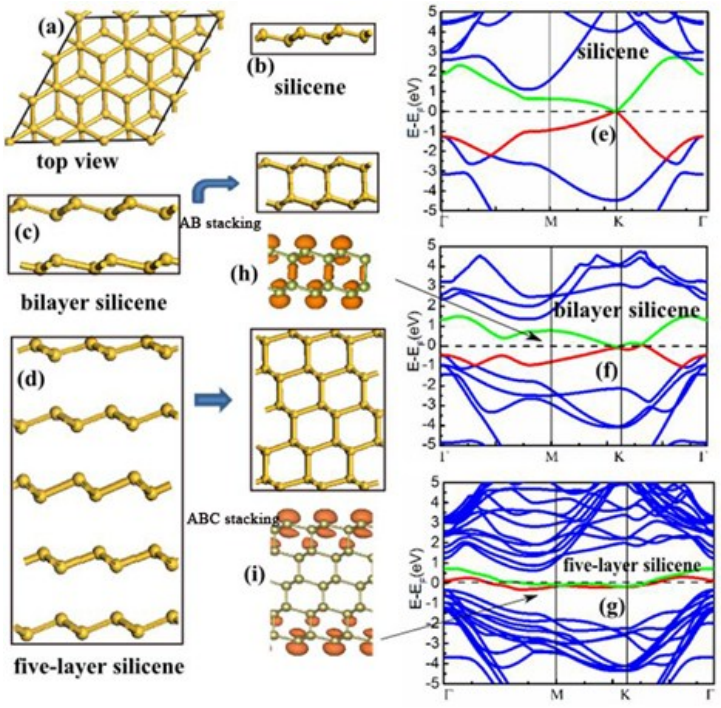

Figure S1 (a) Top view of multilayer silicene. (b - d) Side view of monolayer, bilayer and five-layer silicene. (h-i) Surface dangling bonds distribution on the bilayer and five layer silicon film. (e - f) Energy bonds of monolayer, bilayer and five-layer silicon films.

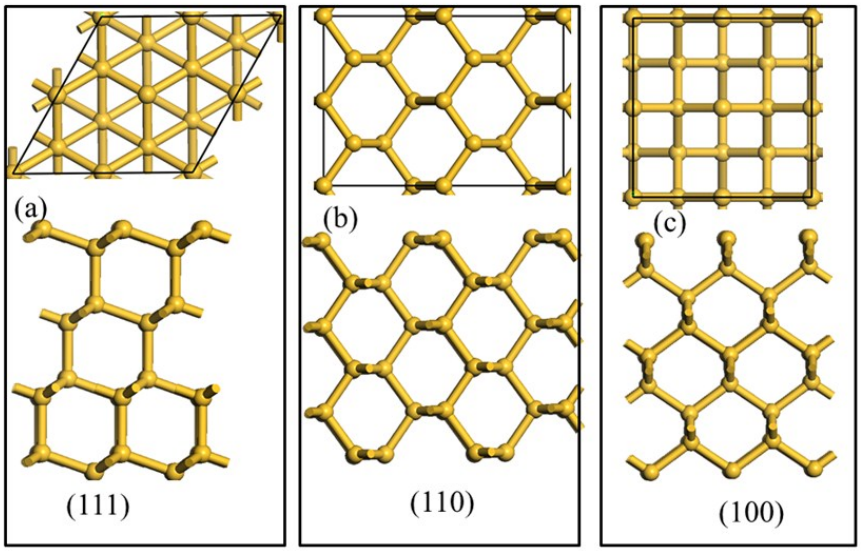

Figure S2 (a - c) Top and side view ultrathin silicon film in the (111), (110) and (100) directions got from the diamond-like bulk silicon.

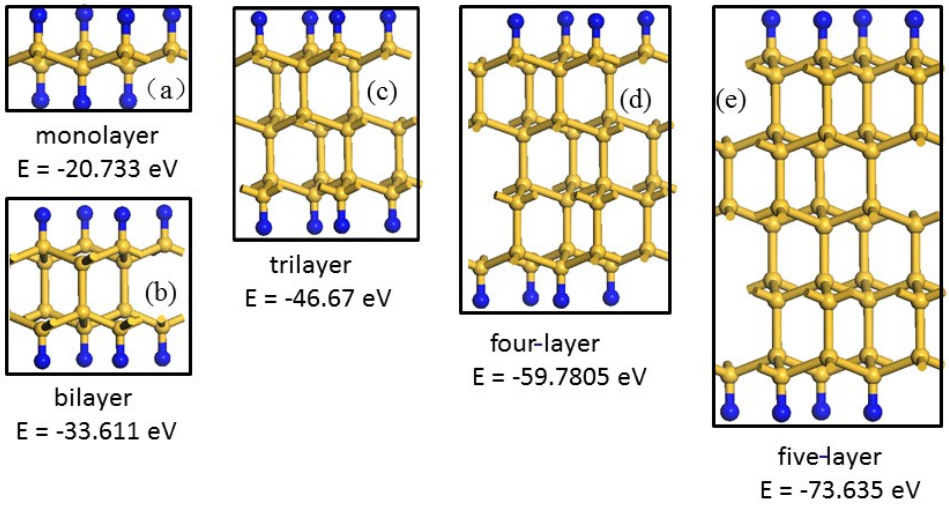

Figure S3 (a - e) Configurations and total energy of monolayer, bilayer, trilayer, four- and five-layer silicon films with surface being decorated hydrogens.

In the following, the lattice vectors and fractional coordinates of the atoms in monolayer, bilayer and five-layer ultrathin silicon films are given.

monolayer:

CIF file

1.00000000000000

3.8872476143104109	0.0000000000000000	0.0000000000000000
-1.9436238071552054	3.3663564339928156	0.0000000000000000
0.0008602010000000	-0.0004966463000000	40.000000000000000000

Si H

2 2

Direct

0.0362873753680049	0.0138976382234901	0.5034428384709315
0.7030408540988518	0.3472830976198438	0.4845372235280294
0.0363327221503980	0.0139323555611739	0.5428871048215598
0.7029890823827500	0.3472468945954930	0.4450927891794905

bilayer:

CIF file

1.00000000000000

3.8738000392999998	0.0000000000000000	0.0000000000000000
-1.9370000361999999	3.3549824770000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	40.0000000000000000

Si H

4 2

Direct

0.0117646159726306	0.0042344914935981	0.4727933718912141
0.3451131936306240	0.6708933333324083	0.4538436377311044
0.0117118366813287	0.0051941931858437	0.5318392242462764

0.6783909279648839 0.3385507432653156 0.5508054721151865
0.6786583699870405 0.3381709420585821 0.5883410017479989
0.3451310507634915 0.6715963356642618 0.4163072852682319

five-layer

CIF file

1.00000000000000

3.8689000607000001 0.0000000000000000 0.0000000000000000

-1.9344500303000001 3.3505657372000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 40.0000000000000000

Si H

10 2

Direct

0.0413056307640147 0.9781227371927841 0.3745931126027031
0.3739022699229082 0.6467408615136208 0.3542175048298049
0.0183937854160732 0.9740096735156243 0.4421127067263910
0.6843803544248814 0.3048240220772911 0.4635079102990787
0.6540275120796366 0.2969418416271736 0.5310559696184782
0.3200642281628632 0.6276993693367956 0.5524283439374145
0.2897452218676548 0.6203298991548536 0.6199635946226181
0.9556832734902514 0.9509818577735132 0.6413547026864990
0.9328012206889795 0.9451176900435740 0.7088739764279026
0.6002022456332199 0.2765065543758851 0.7292644447189431
0.5784316031893226 0.2711425977986153 0.7721901653328445
0.3960826503601851 0.6519428785902690 0.3112876501973147