Electronic Supplementary Material (ESI) for Nanoscale.

Substrate-induced magnetism and topological phase transition in silicene

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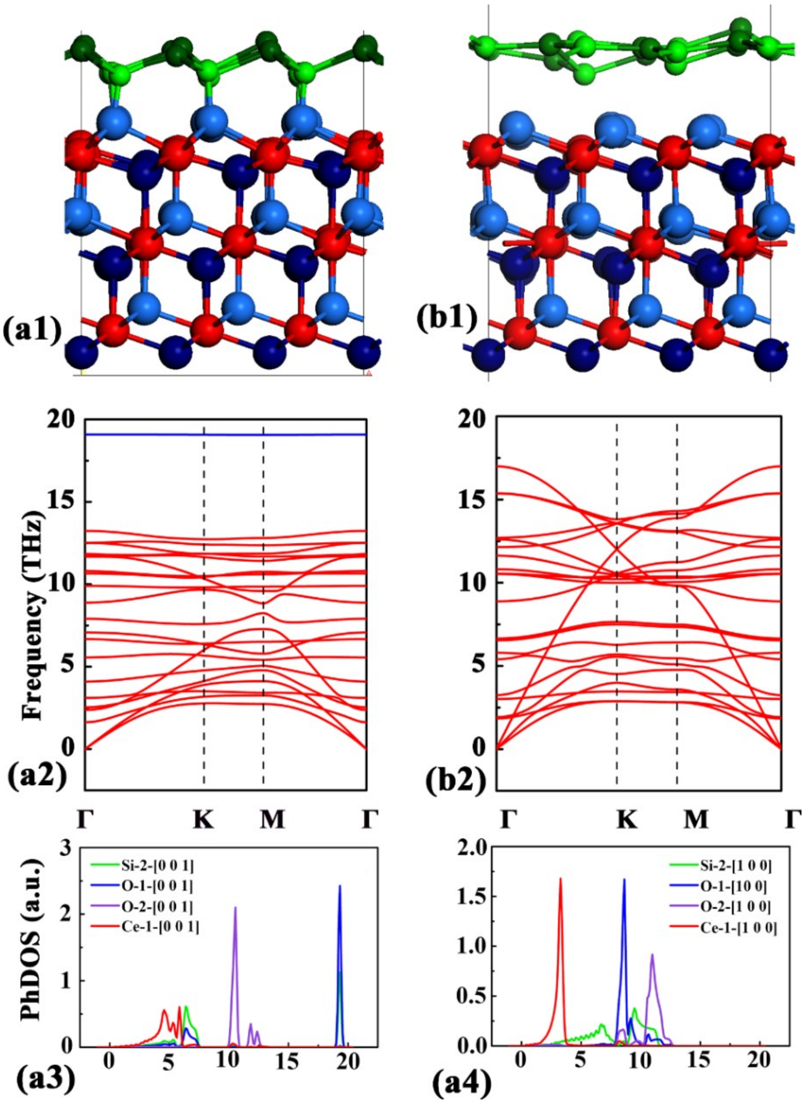

Fig. S1. Thermodynamic stability and bonding characters. (a1, b1) The geometrical structures of covalent bonding CB and non-bonding NB configurations, after 5 ps AIMD simulations at 300 K, suggesting the stability of silicene on CeO$_2$(111) at room. (a2, b2) Phonon dispersions of covalent bonding CB and non-bonding NB configurations. There are no image frequency in these configurations, and the high frequency mode appears in covalent bonding configuration. (a3, a4) The atom-resolved phonon density of states (PhDOS) perpendicular and parallel to the interface for CB configuration.

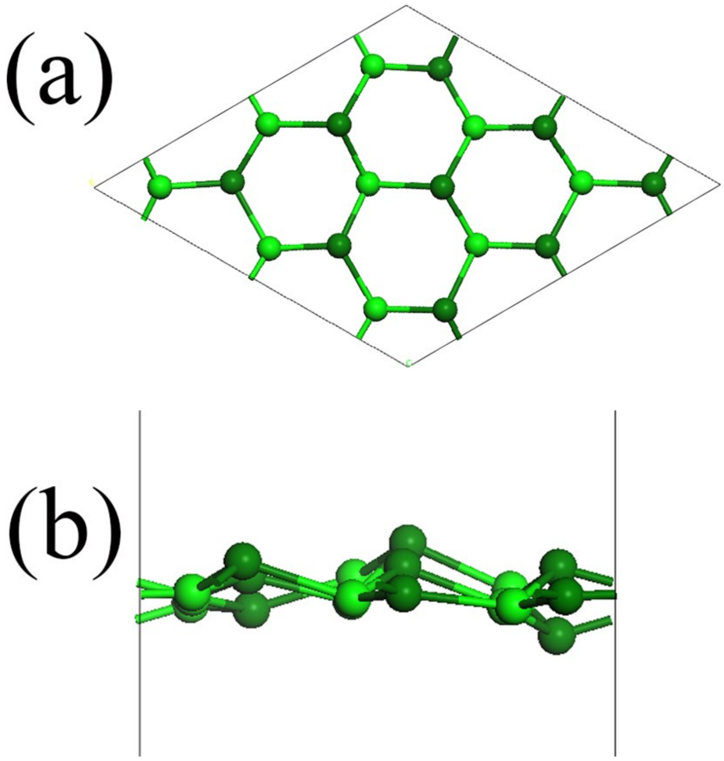

Fig. S2. The geometrical structures of freestanding silicene after 5 ps AIMD simulations at 300 K. (a) and (b) top and side view.

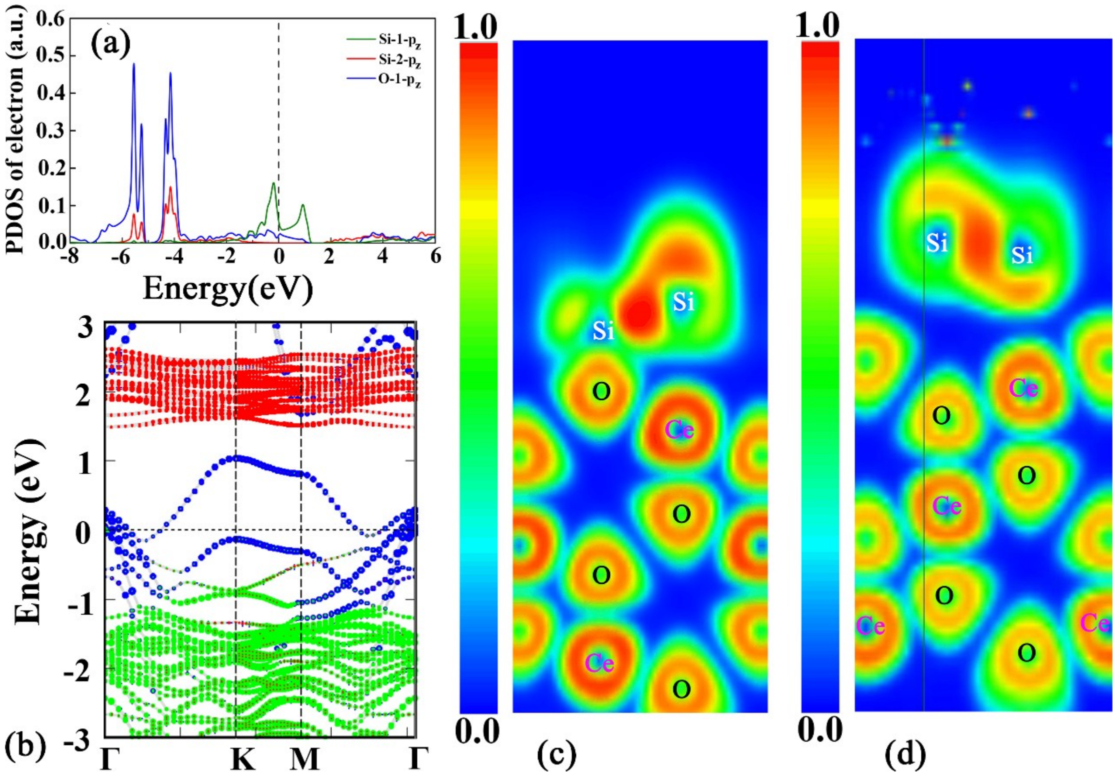

Fig. S3. (a) The partial density of states of electrons of covalent bonding CB configuration. (b) The projected band structure of covalent bonding CB configuration. Red, green and blue symbols represent the projected band dispersion of Ce, O and Si, respectively. (c, d) The contrasting ELFs of covalent bonding CB and non-bonding NB configurations.

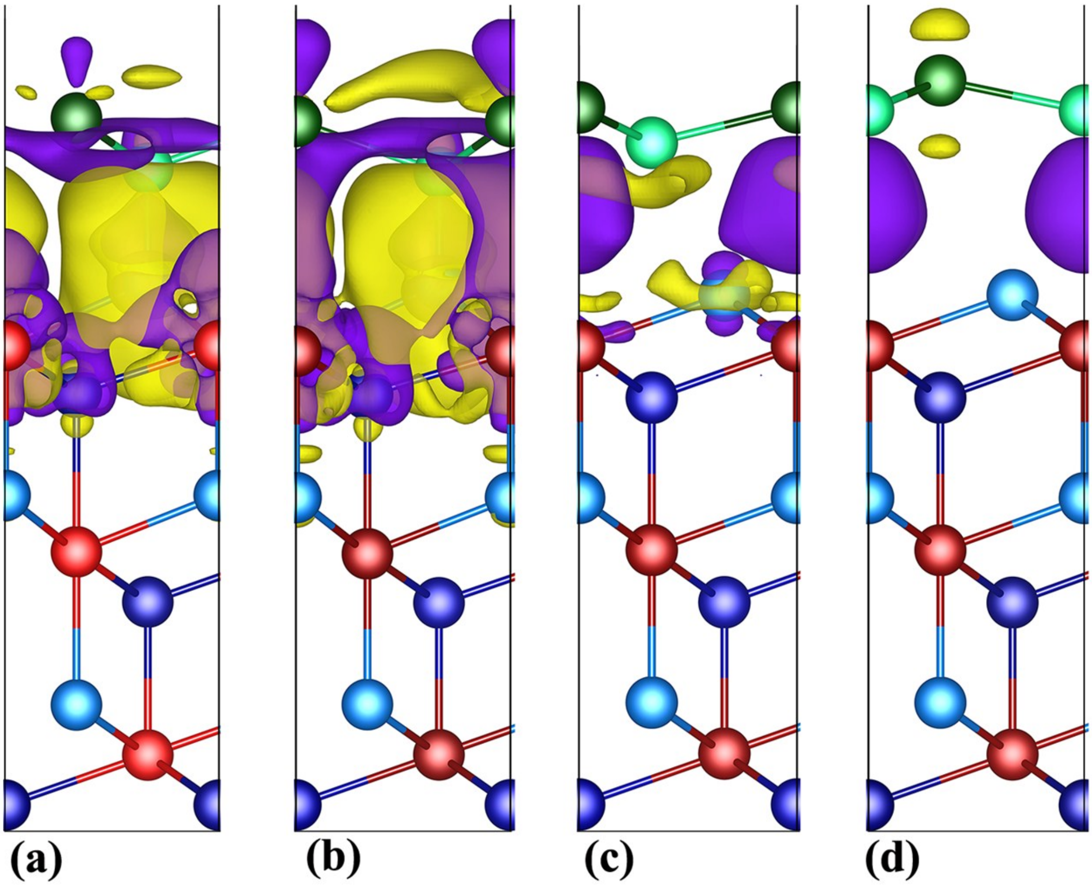

Fig. S4. Three-dimensional charge density differences. (a)-(d) for CA, CB, NA and NB, respectively. Yellow and purple regions denote charge depletion and charge accumulation.

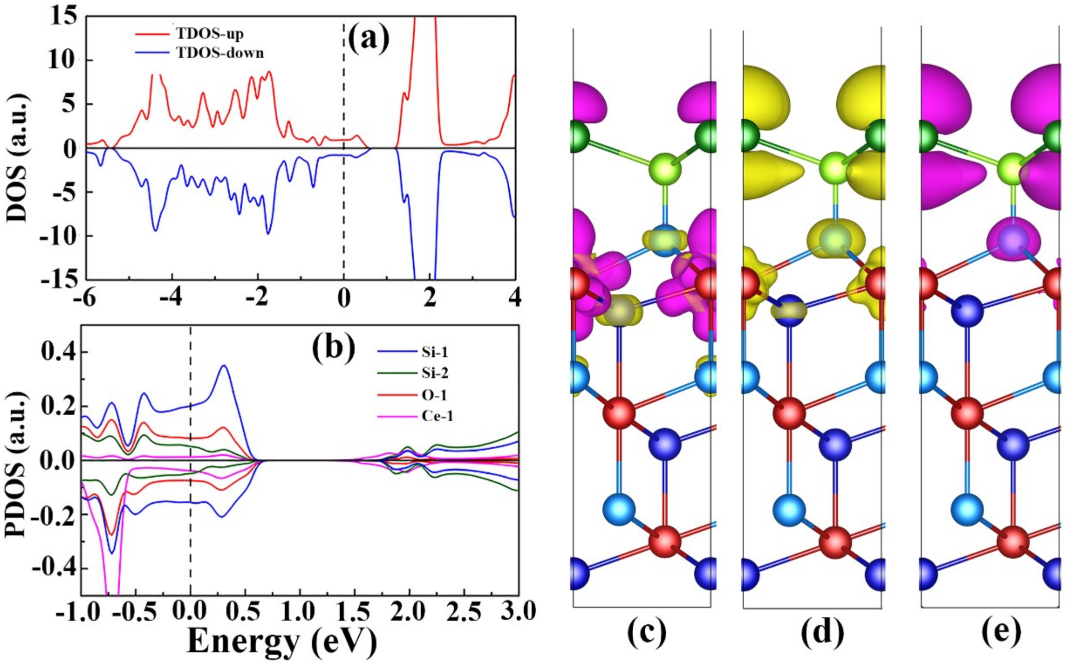

Fig. S5. The electronic structure of covalent bonding CB configuration. (a, b) The spin-polarized total and partial density of states of electrons. (c) Three-dimensional spatial total electron spin-density distribution $\rho_{\uparrow}(\vec{r}) - \rho_{\downarrow}(\vec{r})$. (d, e) The hole spin-density distribution at VB $\rho_{\uparrow}(\vec{r})$ and $\rho_{\downarrow}(\vec{r})$.

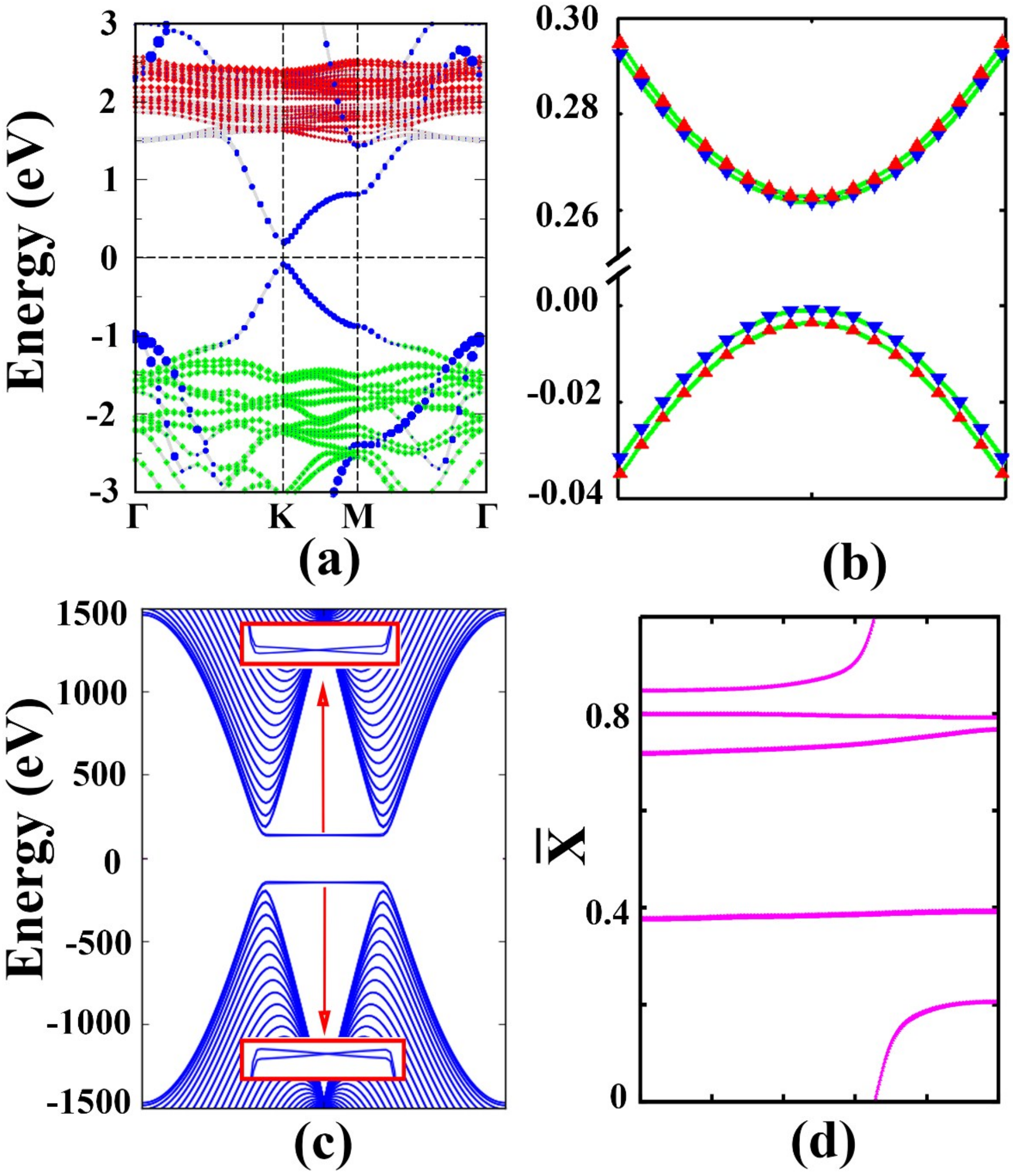

Fig. S6. (a) Projected band structure of non-bonding NB configuration. Red, green and blue symbols represent the projected band dispersion of Ce, O and Si, respectively. (b) Band structures near K point of non-bonding NB configuration. Green solid lines result from tight-binding approach, triangle marks are results of first-principles calculations. (c) Band structure of zigzag nanoribbon of silicene on CeO_2 (111) corresponding to NB configuration. There are no edge crossing to fermi level. (d) The evolution of the charge centers of the Wannier functions of silicene on CeO_2(111), implying the Z_2 invariant is zero.

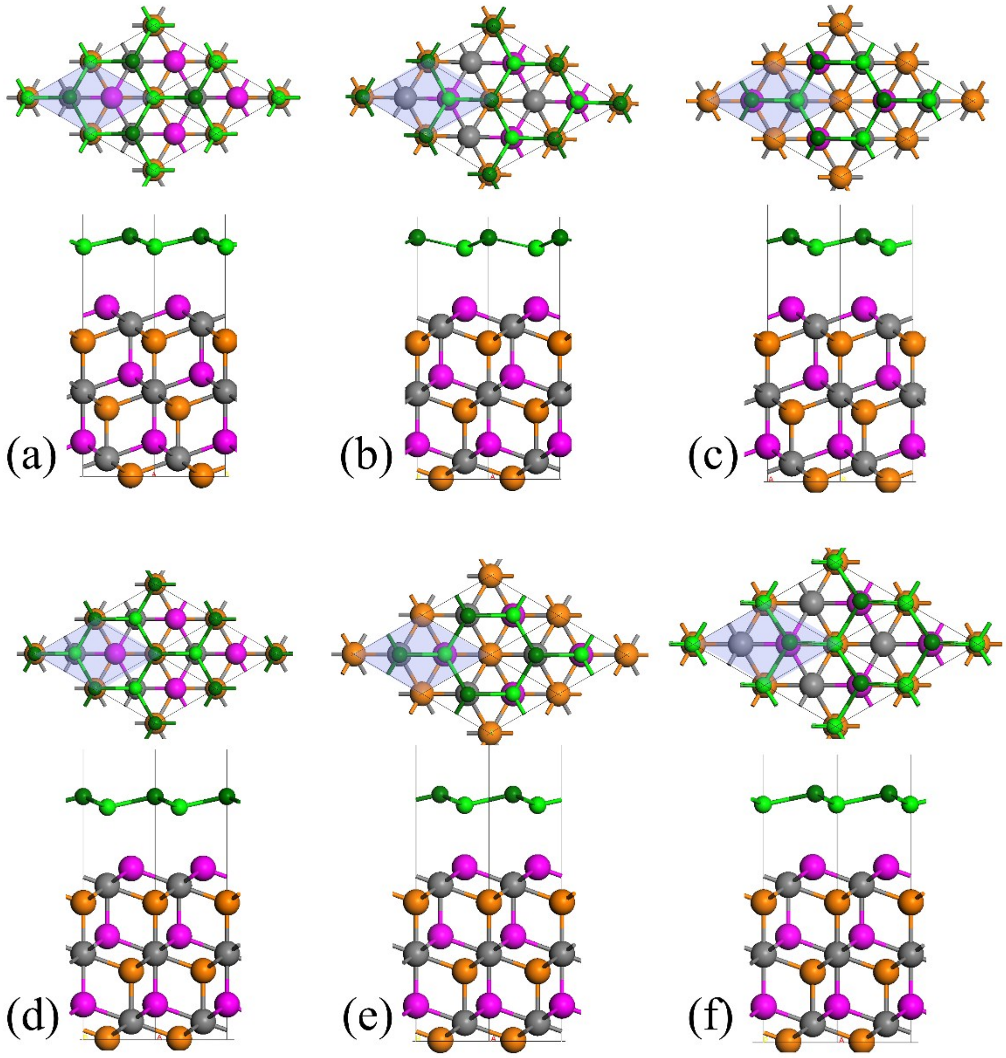

Fig. S7. Silicene on CaF_2 (111). (a-f) Six different configurations of silicene/CaF_2 (111). Gray spheres represent Ca atoms, dark green and light green spheres represent up and down half-layer Si atoms of silicene, and pink and orange spheres represent F atoms.

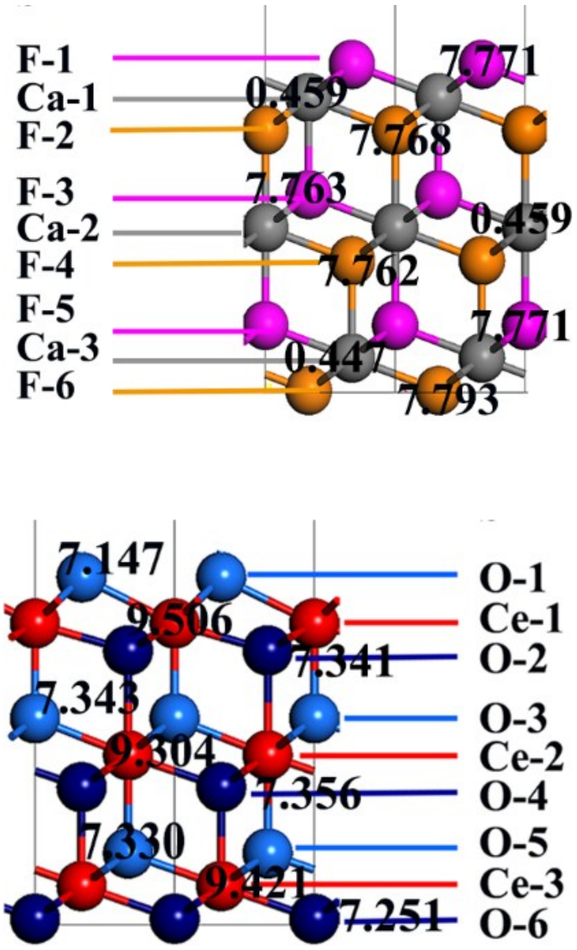

Fig. S8. The Bader charge of each atom for clean CeO_2 (111) and CaF_2 (111).

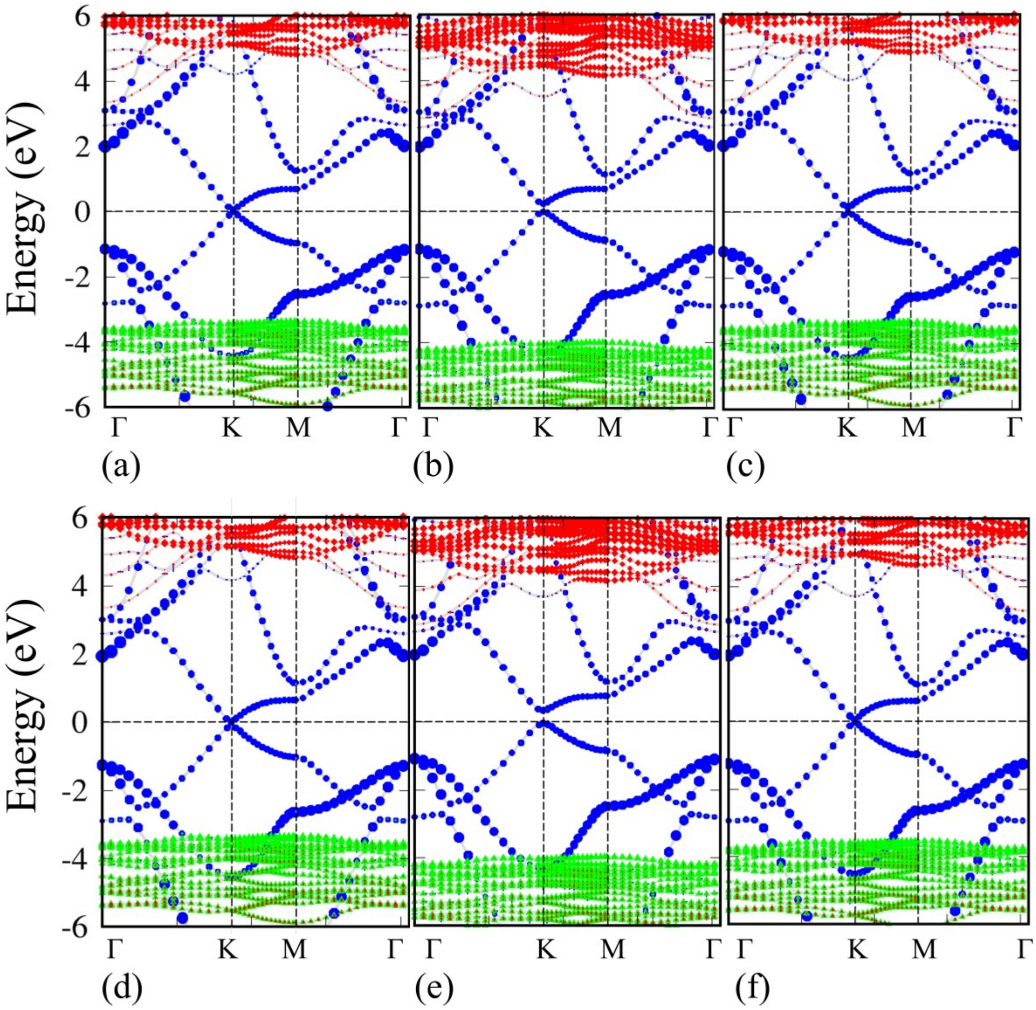

Fig. S9. (a-f) Band structures for silicene/CaF_2 (111) corresponding to six configurations (a-f) in Fig. S7. Red, green and blue dot represent the projected band dispersion of Ca, F and Si.

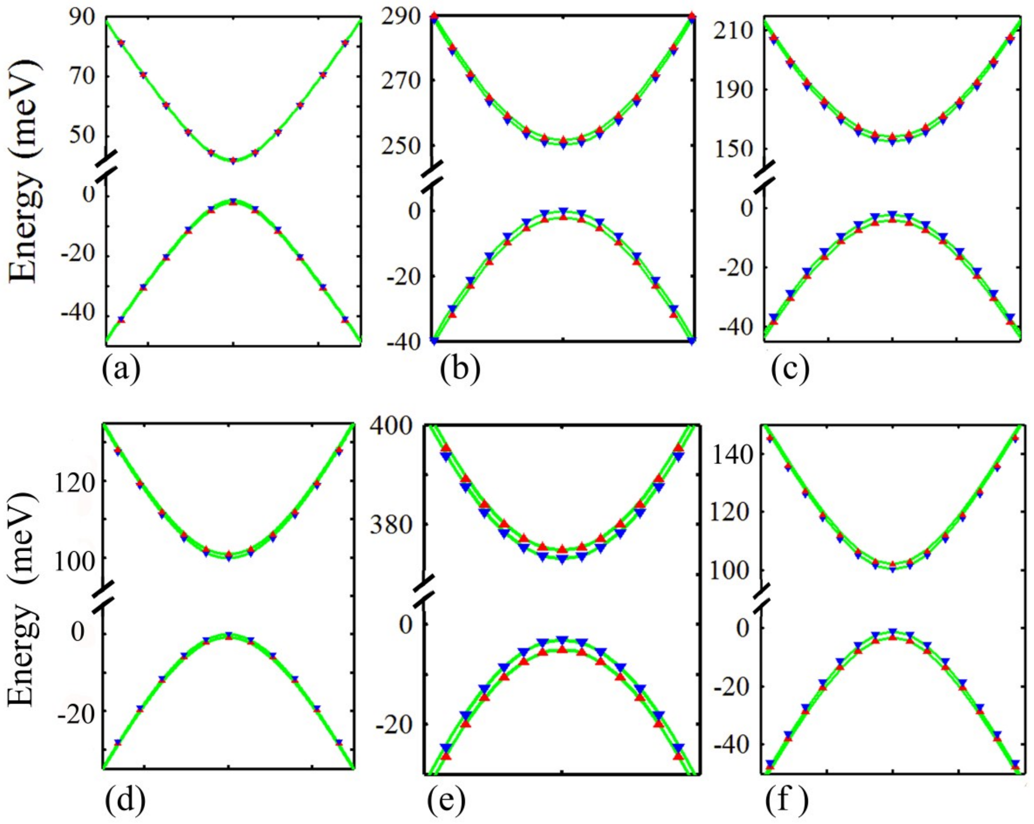

Fig. S10. (a-f) Band structures near K point of six configurations of silicene/CaF_2(111) corresponding to six configurations (a-f) in Fig. S7. Green solid lines denote the result from tight-binding approach, triangle symbols are results of first-principles calculations.

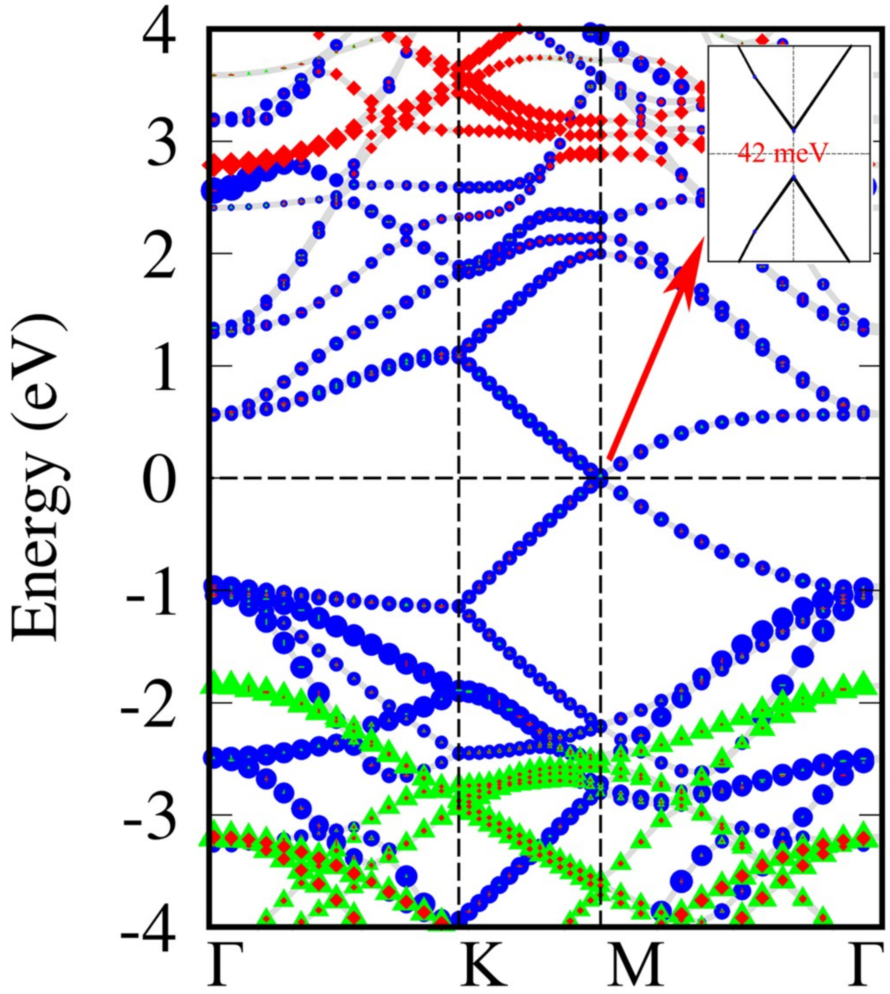

Fig. S11. Band structure for silicene/BN. Red, blue and green symbols represent the projected band dispersion of B, N and Si.

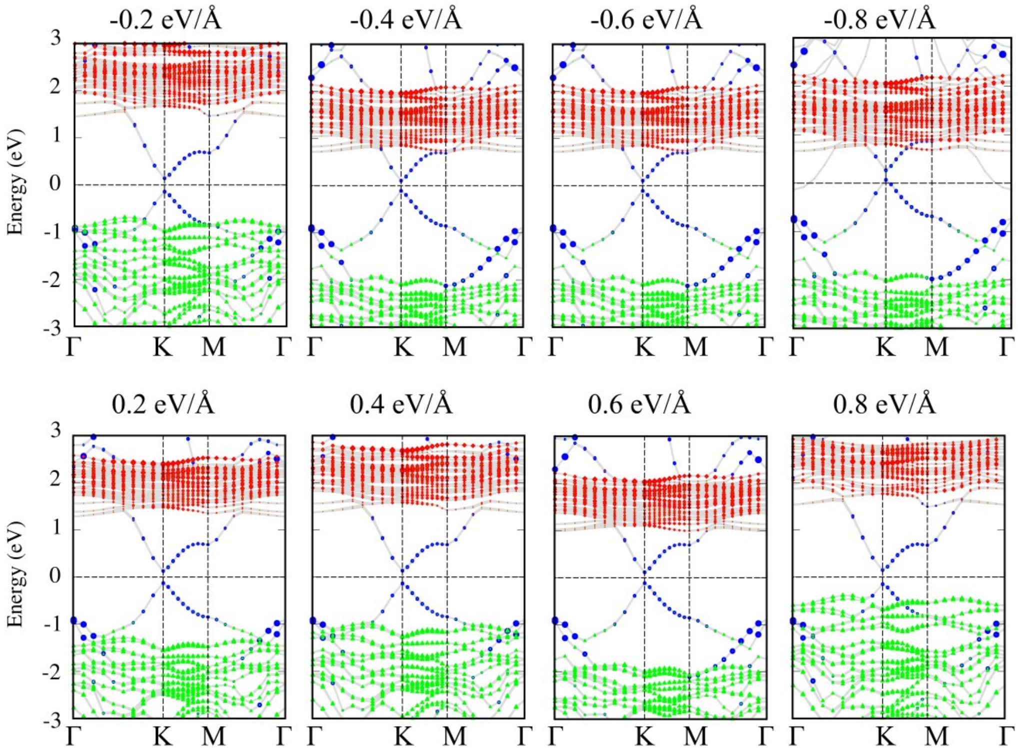

Fig. S12. The band structures of silicene/CeO_2 (111) corresponding to NA configuration under various vertical external fields. Red, green and blue symbols represent the projected band dispersion of Ce, O and Si. Here, positive value denotes the direction of electric field from CeO_2 (111) to silicene, while negative value presents reverse direction of electric field.

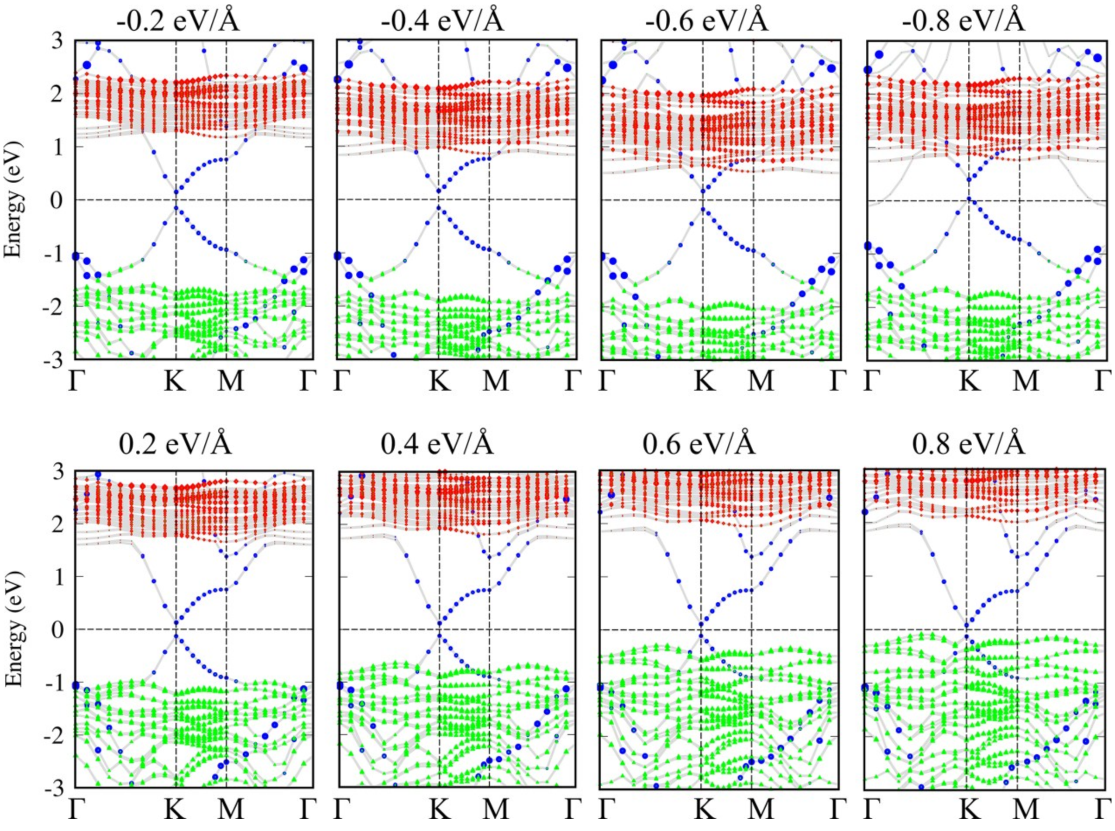

Fig. S13. The band structures of silicene/CeO_2(111) corresponding to non-bonding NB configuration under various vertical external fields. Red, green and blue symbols represent the projected band dispersion of Ce, O and Si. Here, positive value denotes the direction of electric field from CeO_2 (111) to silicene, while negative value presents reverse direction of electric field.

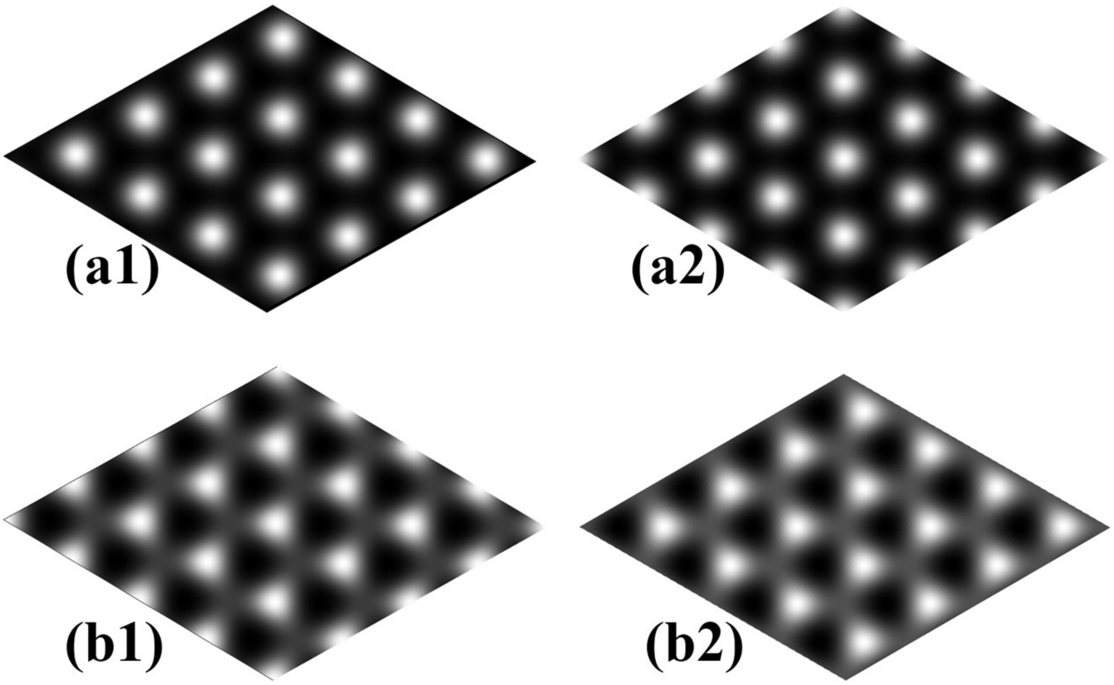

Fig. S14. Simulated scanning tunneling microscopy (STM) images of 4 × 4 supercell of silicene on CeO_2 (111), (a1) and (a2) the covalent bonding configurations for CA and CB; (b1) and (b2) the non-bonding configurations for NA and NB. All images were simulated using a bias voltage of -3.0 V relative to the Fermi energy. Obviously, the results predict the bonding and non-bonding configurations can been directly identified by STM measuration.

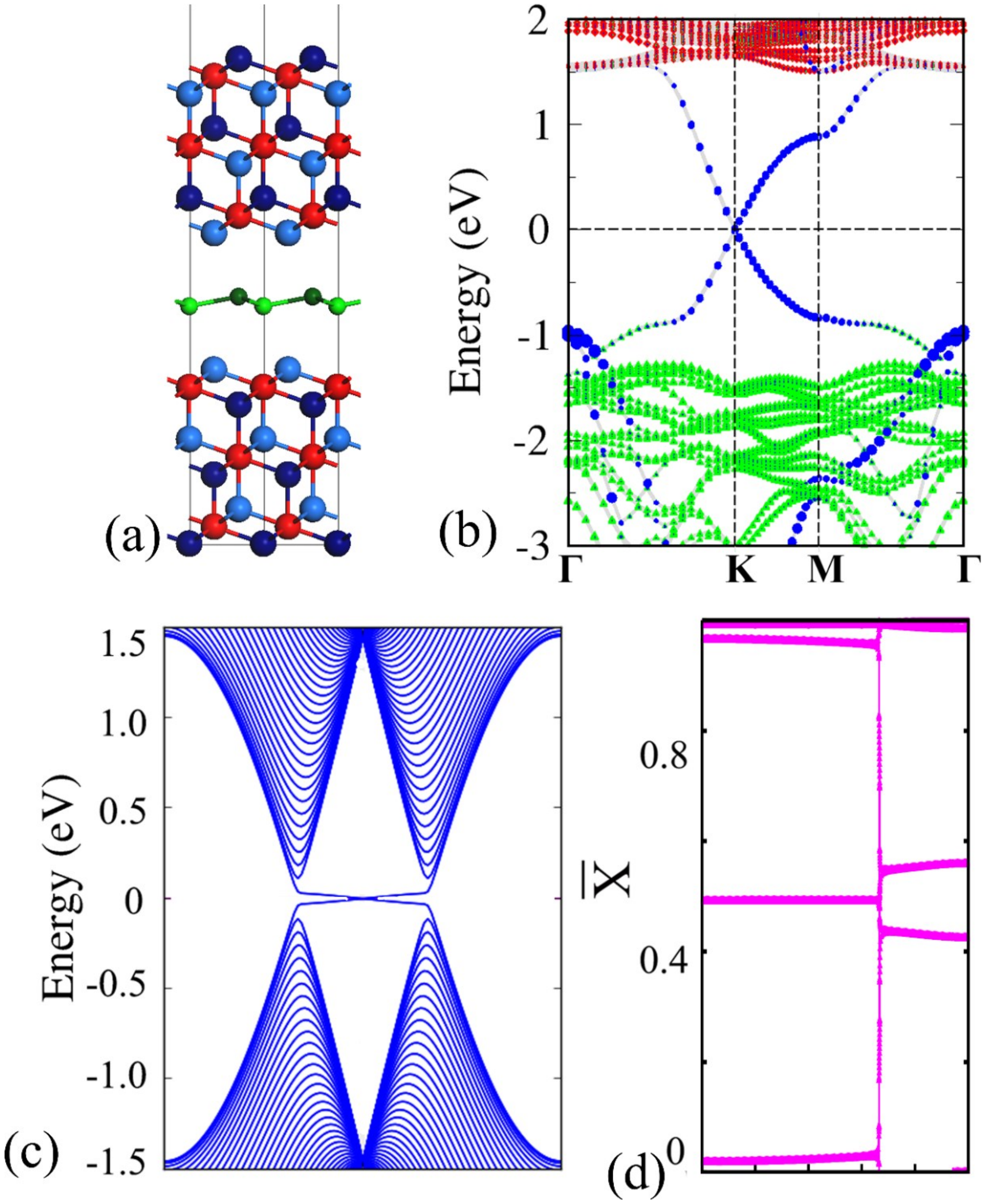

Fig. S15. Geometry, electronic structures and topological properties of inverse symmetrical sandwich structure corresponding to NB configuration. (a) The geometrical structure. Red spheres represent Ce atoms, dark green and light green spheres represent the upper and lower layer Si atoms of silicene, and dark blue and light blue spheres represent O atoms. (b) Band structures. Red, green and blue symbols represent the projected band dispersion of Ce, O and Si. (c) Band structure of zigzag nanoribbon of silicene in CeO_2 (111)/silicene/CeO_2 (111). (d) The evolution of the charge centers of the Wannier functions, implying the Z_2 invariant is one.

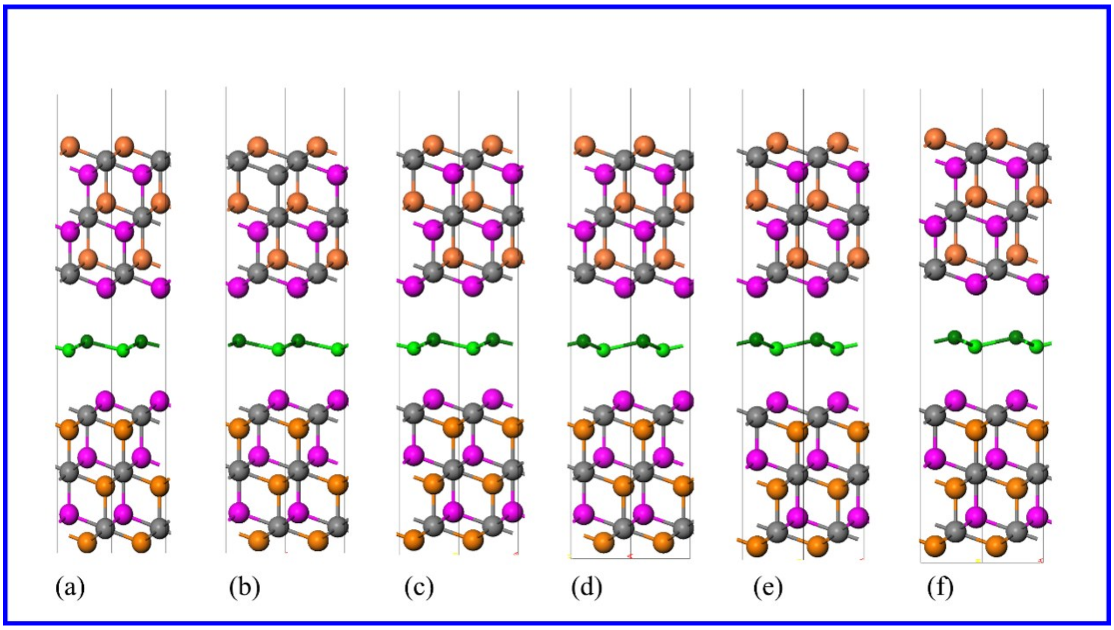

Fig. S16. (a-f) Geometry for six different configurations of CaF_2(111)/silience/CaF_2(111). Gray spheres represent Ca atoms, dark green and light green spheres represent the upper and lower layer Si atoms of silicene, and pink and orange spheres represent F atoms.

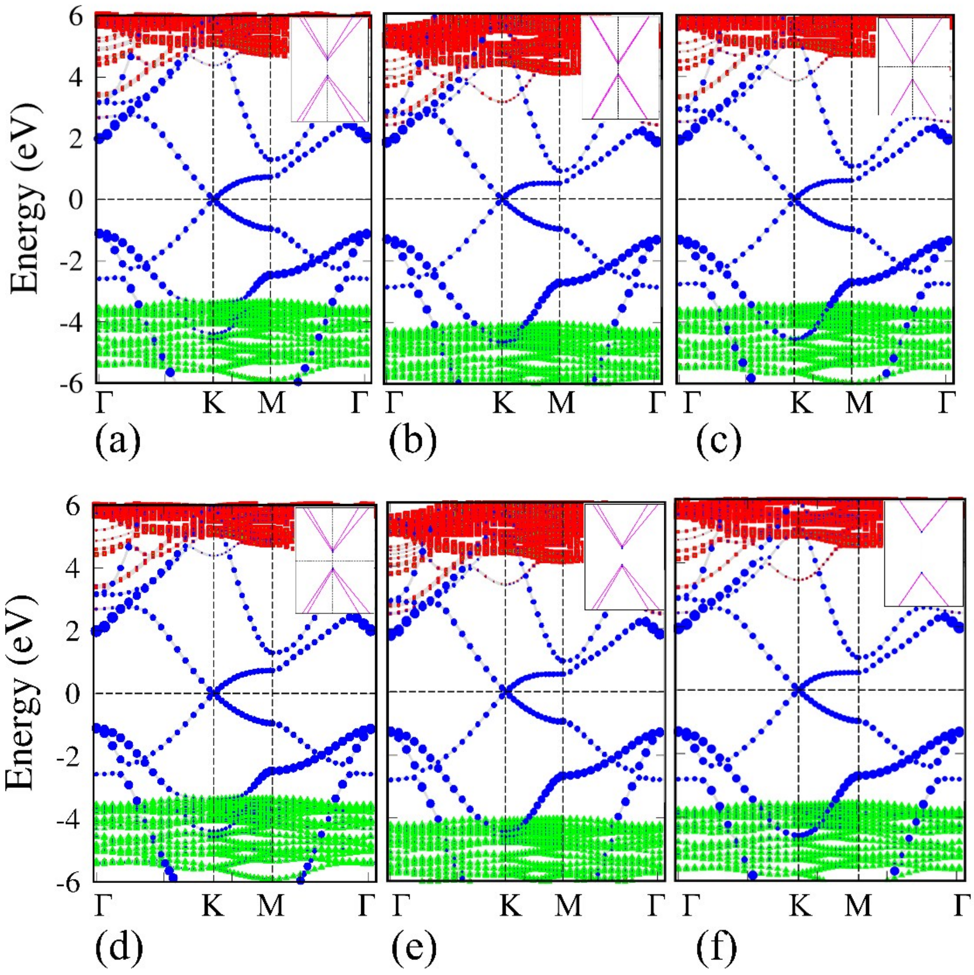

Fig. S17. (a-f) Band structures of $CaF_2(111)$/silicene/$CaF_2(111)$ corresponding to six configurations (a-f) in Fig. S16. Red, green and blue symbols represent the projected band dispersion of Ca, F and Si.

TABLE S1. Silicene on the CaF_2 (111) surface. The E_b is the binding energy per Si atom. The E_g is the gap calculated at the K point. The Hamiltonian parameters defined in Eqs. (1) are given in meV. The b is the separation between the upper and lower layer silicene. The d is the interfacial distance between silicene and substrate.

	E_b(meV)	E_g(meV)	γ_m	γ_{so}	γ_{R1}	γ_B	b (Å)	v_F (10^5m/s)	d (Å)
a	270.2	44.4	21.87	0.33	0.20	-0.12	0.47	5.38	2.75
b	249.7	253.7	125.97	0.88	1.26	-0.12	0.50	5.36	2.85
c	207.9	158.1	78.17	0.88	0.49	-0.07	0.43	5.48	3.08
d	237.3	91.7	45.40	0.45	0.35	0.05	0.43	5.46	2.95
e	272.1	379.9	189.02	0.93	2.67	-0.07	0.51	5.41	2.76
f	219.3	102.2	50.12	0.98	0.59	-0.12	0.45	5.47	2.99