Supplementary material

Tunable and sizable band gap in silicene by surface adsorption

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Methods

The spin-orbital coupling (SOC) effects are investigated by using the plane wave (PW) basis set and the projector-augmented wave (PAW) pseudopotential implemented in the VASP package.[1] Generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) form is employed for the exchange-correlation functional.[2] A PW energy cutoff of 500 eV and a 45 × 45 × 1 Monkhorst-Pack *k*-mesh[3] are used to generate the charge densities.

The quasiparticle calculations are carried out using the ABINIT package.[4] First, we compute the wave functions using DFT. The local density approximation (LDA) of the Ceperley-Alder form is employed for the exchange-correlation functional.[5] A PW energy cutoff of 500 eV is used, together with the norm-conserving pseudopotentials,[6] and the Brillouin zone is sampled with an 18 × 18 × 1 Monkhorst-Pack grid.[3] Second, the quasiparticle energies E_{nk} are calculated using the following quasiparticle Schrödinger equation, which uses the self-energy Σ acquired from the *GW* approximation.[7]

$$[-\frac{\nabla^2}{2}+V_{\text{ion}}+V_{\text{Hartree}}+\sum(E_{nk})]\Psi_{nk}=E_{nk}\Psi_{nk} \qquad (1)$$

Therein, the Green function and the Coulomb screening are constructed from the LDA results in the first step, and the plasmon–pole model is used for the screening computation. We perform the *GW* calculation in a nonself-consistent way.

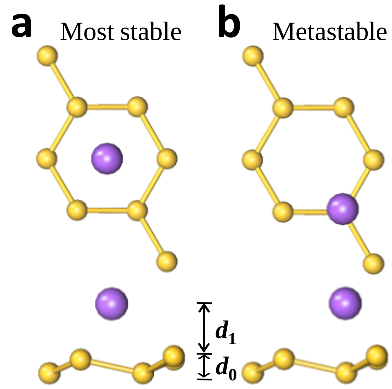

Figure S1: Possible configurations of $AMSi_8$ monolayer. The AM atom is above the hexagon center in the most stable state of $AMSi_8$ monolayer and above one of the lower Si atom in the metastable state.

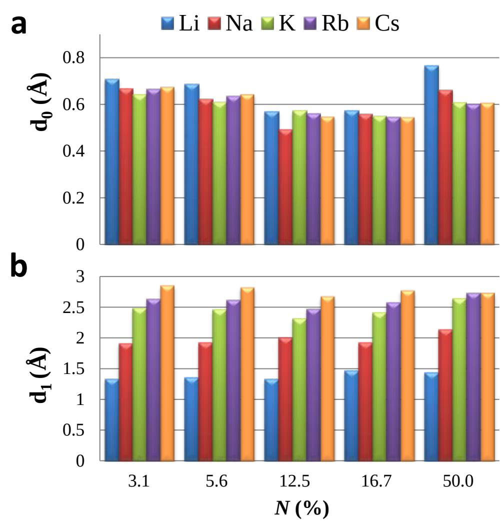

Figure S2: Dependences of the silicene buckling d_0 and the distance between the AM atom and silicene d_1 on the AM coverage. d_0 of the pure silicene is 0.46 Å.

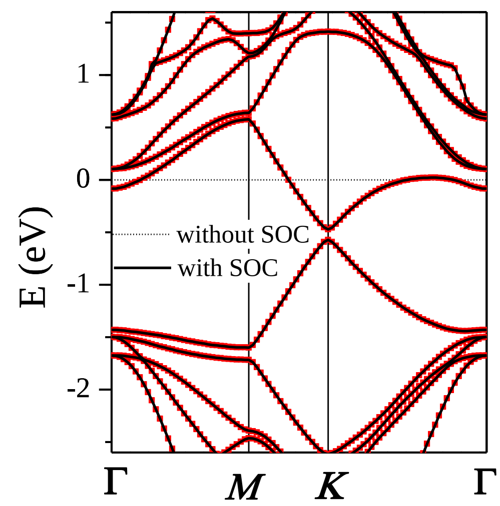

Figure S3: Band structures of $NaSi_8$ monolayer with and without the inclusion of the SOC effects. In order to keep consistency and obtain a reliable compared result, all the above band structures are calculated by using the PW basis set implemented in the VASP package. The band gap of $NaSi_8$ monolayer with the inclusion of the SOC effects is 0.1 eV, which is only 1.2 meV larger than the one without the inclusion of the SOC effects.

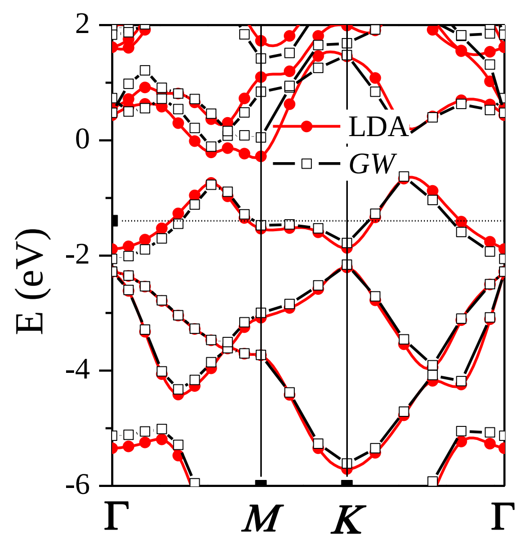

Figure S4: Band structures of $NaSi_2$ monolayer at the LDA and *GW* levels. For the sake of comparison, both the band structures are calculated by using the PW basis set implemented in the ABINIT package.

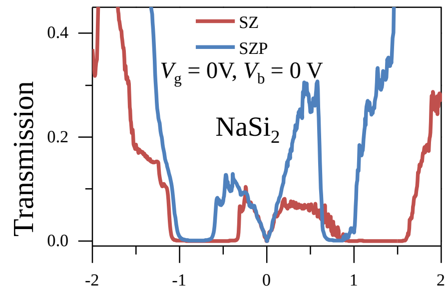

Figure S5: Transmission spectrum of the Na-covered silicene FET with N = 50%. The channel is 113.8 Å long. A smaller transport gap is obtained in the transmission spectrum by using the SZP basis set compared with the SZ basis set. Both V_g and V_b are set to zero.

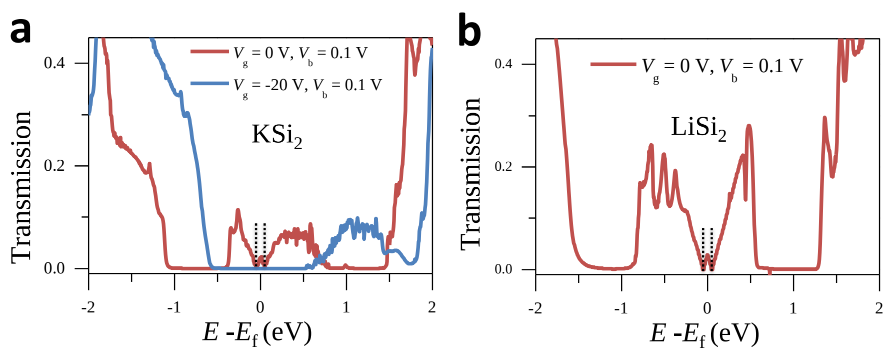

Figure S6: Transmission spectra of the AM-covered silicene FET. The channel is composed of (**a**) K-covered or (**b**) Li-covered silicene with N = 50.0%. The channel is 113.8 Å long. The SZ basis set is used. The vertical dashed-line indicates the bias window.

References

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