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Supplementary Materials

Tunable Band Gap and Doping Type in Silicene by Surface Adsorption: towards Tunneling Transistors

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Parameters of Theoretical Calculations

In our study, the spin-orbital coupling (SOC) effects[1] are investigated by density functional theory, using the plane wave (PW) basis set and the projector-augmented wave (PAW) pseudopotential implemented in the Vienna *ab-initio* Simulation Package (VASP)[2]. The generalized gradient approximation (GGA) functional of the Perdew–Burke–Ernzerhof (PBE) form[3] is adopted. The cut off energy is set to 450 eV after convergence tests. An equivalent Monkhorst-Pack (MP) *k*-point grid[4] of 36 × 36 × 1 in one primitive cell is chosen for supercell relaxation and 40 × 40 × 1 for supercell static calculations. A vacuum layer of 15 Å is fixed to avoid periodic interaction. Dipole corrections perpendicular to the silicene plane is engaged in all calculations. In the G_0W_0 calculation of $PtSi_8$, the PBE pseudopotentials designed for *GW* calculations is employed. The equivalent *k*-point grid is changed to 24 × 24 × 1 in order to reduce memory consumption without losing much accuracy. In the response function calculation, the optical spectra method [5] is used together with energy cutoff of 200 eV and 512 bands. In the quasi-particle energy calculation, 100 bands are used.

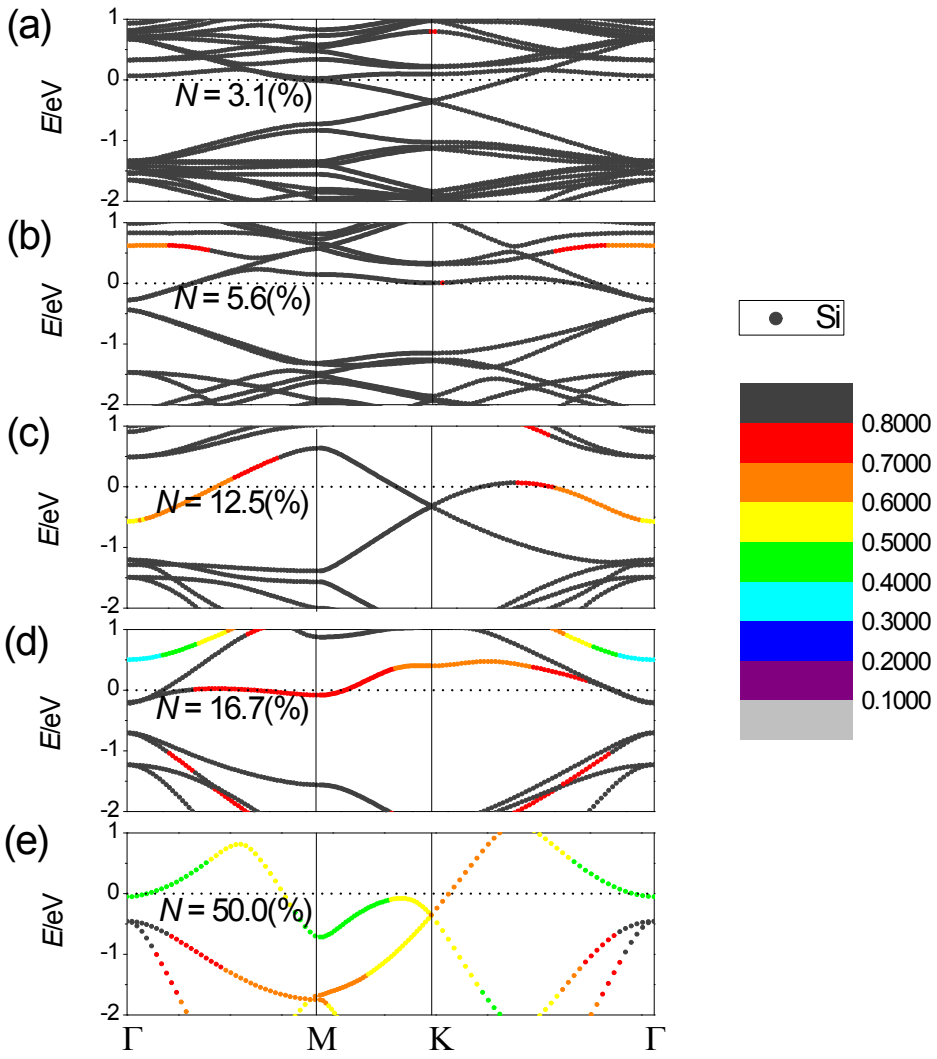

Fig. S1: (a-e) Electronic band structures of the Ag-covered silicene at coverages of N = 3.1%, 5.6%, 12.5%, 16.7%, and 50.0%, respectively. The Fermi level is set to zero. Contributions from the silicon atoms are marked as different color proportional to the weight.

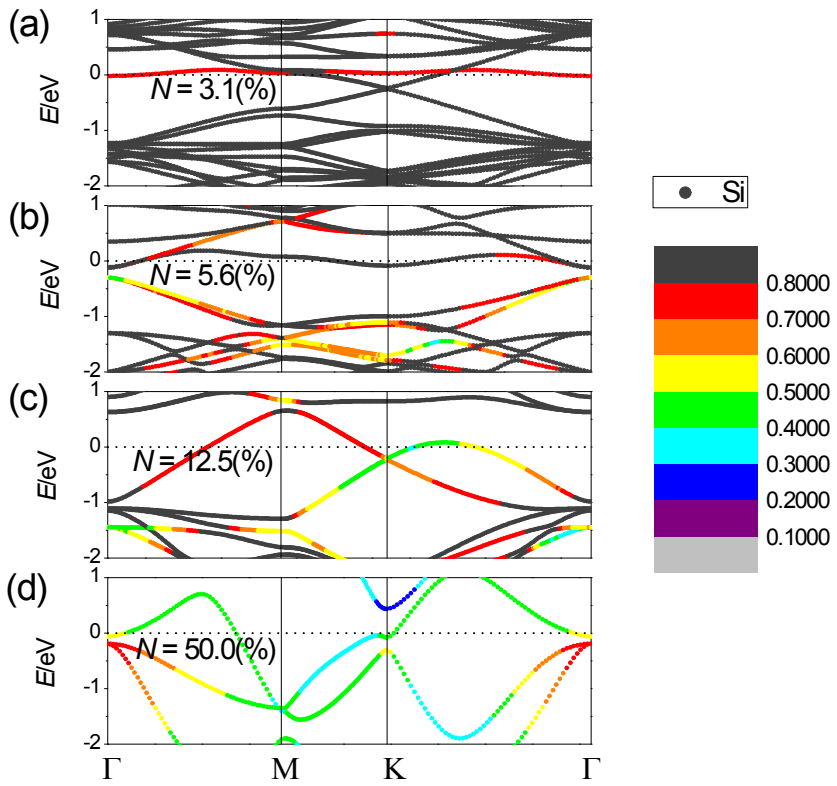

Fig. S2: (a-d) Electronic band structures of the Au-covered silicene at coverages of N = 3.1%, 5.6%, 12.5%, and 50.0%, respectively. The Fermi level is set to zero. Contributions from the silicon atoms are marked as different color proportional to the weight.

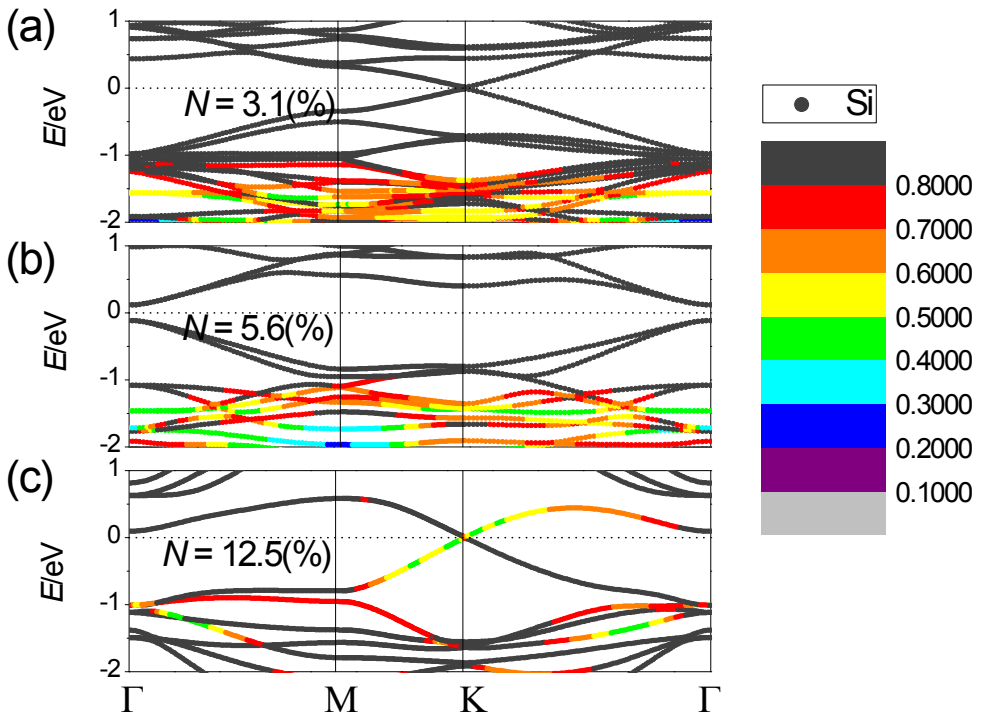

Fig. S3: (a-c) Electronic band structures of the Pt-covered silicene at coverages of N = 3.1%, 5.6%, and 12.5%, respectively. The Fermi level is set to zero. Contributions from the silicon atoms are marked as different color proportional to the weight.

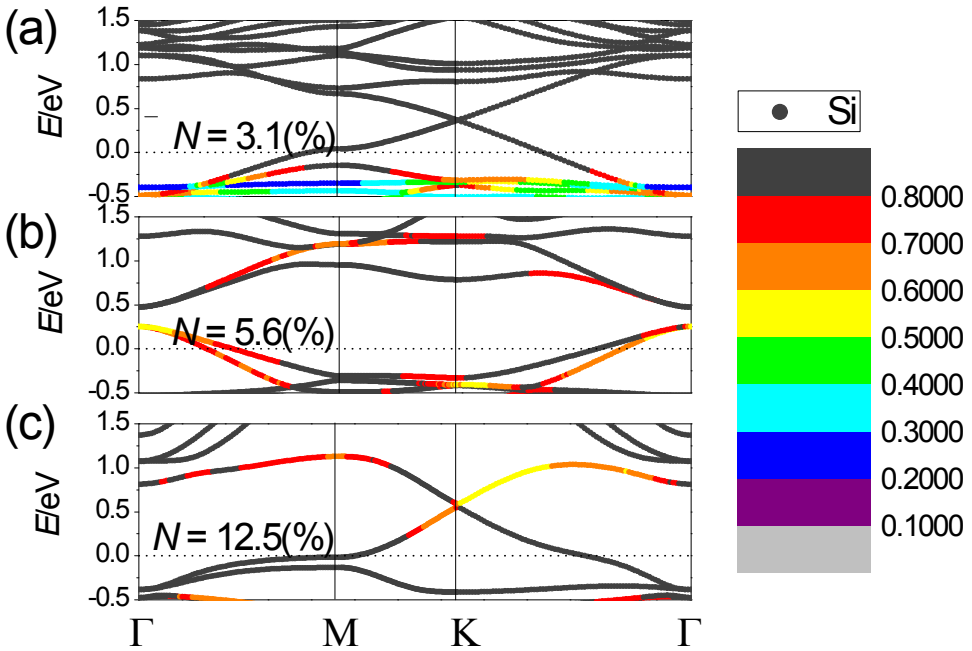

Fig. S4: (a-c) Electronic band structures of the Ir-covered silicene at coverages of N = 3.1%, 5.6%, and 12.5, respectively. The Fermi level is set to zero. Contributions from the silicon atoms are marked as different color proportional to the weight.

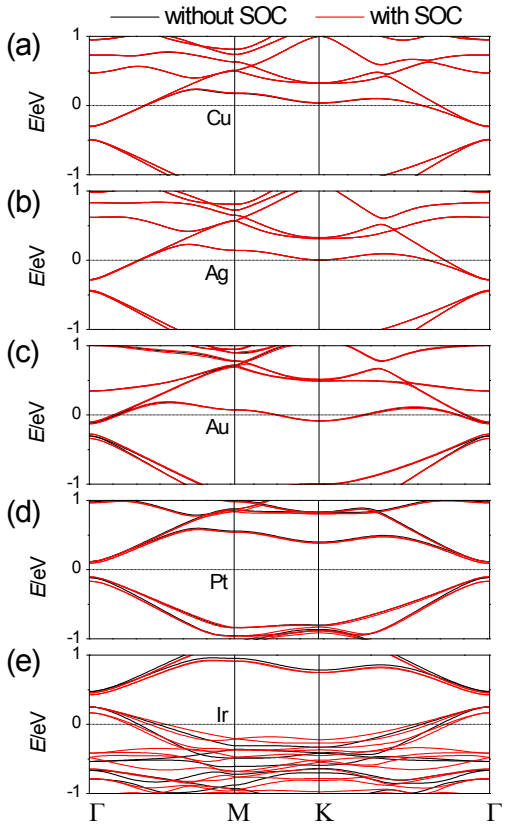

Fig. S5: Electronic band structures of (a) Cu, (b) Ag, (c) Au, (d) Pt, and (e) Ir-covered silicene with and without the inclusion of the SOC effects at the coverage of N = 5.6%. In order to get reliable results, all the above band structures are calculated by using the PAW basis set completed in the VASP package. The band gap of $CuSi_{18}$ with the inclusion of the SOC effects is 0.186 eV, which is only 0.7 meV smaller than the one without the inclusion of the SOC effects. The underestimation to the band gap for Ag, Au, Pt, and Ir-covered silicene are 7, 30, 30, and 44 meV, respectively.

Fig. S6: Top view of (a) Free-standing silicene electron densities at the Dirac point. (b)-(c) Electron densities of the valence band maximum and conduction band minimum in Cu-covered silicene at with coverage of N = 12.5% and 50.0%, respectively. The isovalue is 0.03 e/Å^3.

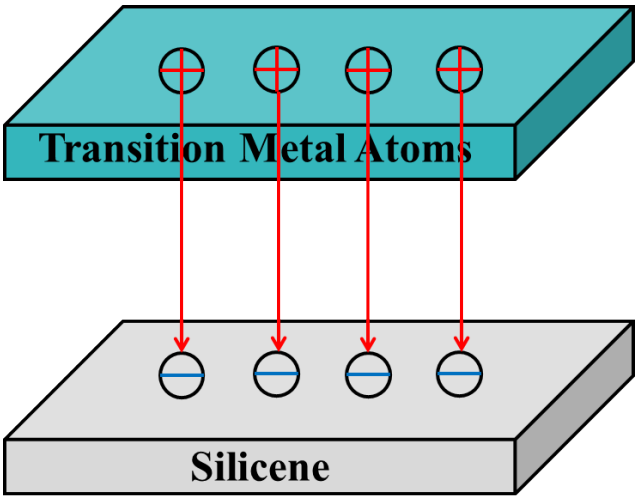

Fig. S7: Schematic of the parallel plate capacitor model. *E* denotes the electric field between transition metal and silicene.

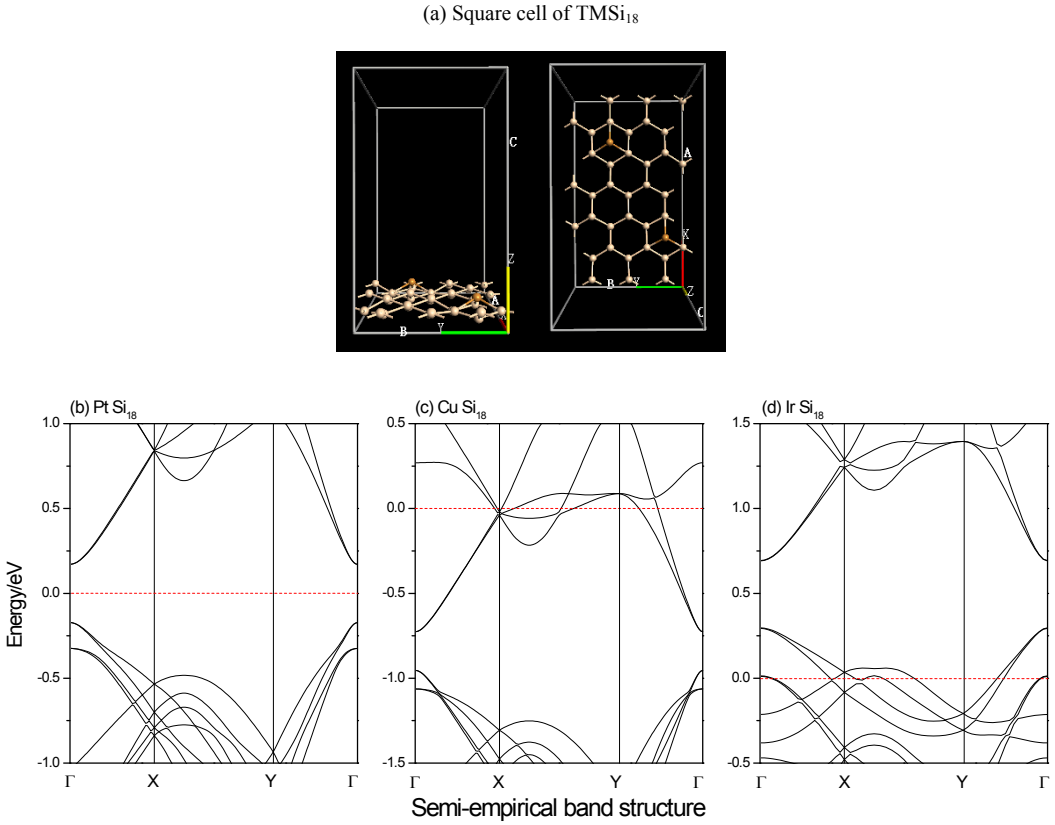

Fig. S8: (a) Square cell of $TMSi_{18}$ used in transport calculation. (b)-(d) The semi-empirical band structure of $TMSi_{18}$ (TM = Pt, Cu, and Ir). The gap sizes and doping type by the SE approach are in coordinate with those by the DFT approach in Fig. S5.

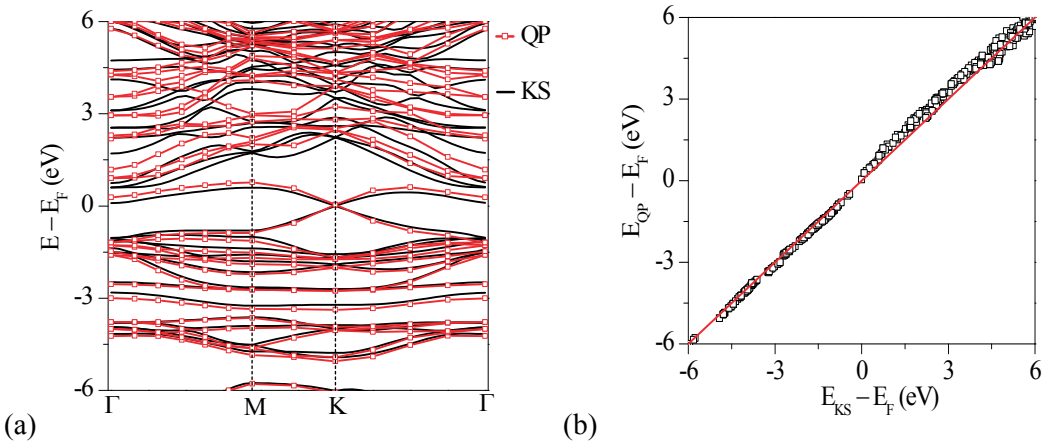

Fig. S9: (a) Quasi-particle (QP) and Kohn-Sham (KS) band structures of $PtSi_8$ by the G_0W_0 and DFT approach. The band gap changes from 0.02 eV in DFT to zero in G_0W_0. (b) Comparison between QP energies and KS energies. The points are close to 1:1 (red line), especially for those near E_f, which suggests that the QP corrections do not significantly affect our results and conclusions.

References

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