Supplementary Materials

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

Zeyuan Ni,1,† Hongxia Zhong,1,† Xinhe Jiang,1,† Ruge Quhe,1,3 Guangfu Luo,4 Yangyang Wang,† Meng Ye,1 Jinbo Yang,1,2,* Junjie Shi,1,* and Jing Lu1,2,*

1State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China
2Collaborative Innovation Center of Quantum Matter, Beijing 100871, China
3Academy for Advanced Interdisciplinary Studies, Peking University, Beijing 100871, China
4Materials Science and Engineering Department, University of Wisconsin-Madison, Wisconsin 53706, United States
†These authors contributed equally to this work.
*Corresponding author: jinglu@pku.edu.cn, jjshi@pku.edu.cn, jbyang@pku.edu.cn

Parameters of Theoretical Calculations

In our study, the spin-orbital coupling (SOC) effects1 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) form3 is adopted. The cut off energy is set to 450 eV after convergence tests. An equivalent Monkhorst-Pack (MP) k-point grid4 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 G0W0 calculation of PtSi8, 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 $0.03 \, \text{e/Å}^3$. 
Fig. S7: Schematic of the parallel plate capacitor model. $E$ denotes the electric field between transition metal and silicene.

(a) Square cell of TMSi$_{18}$

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