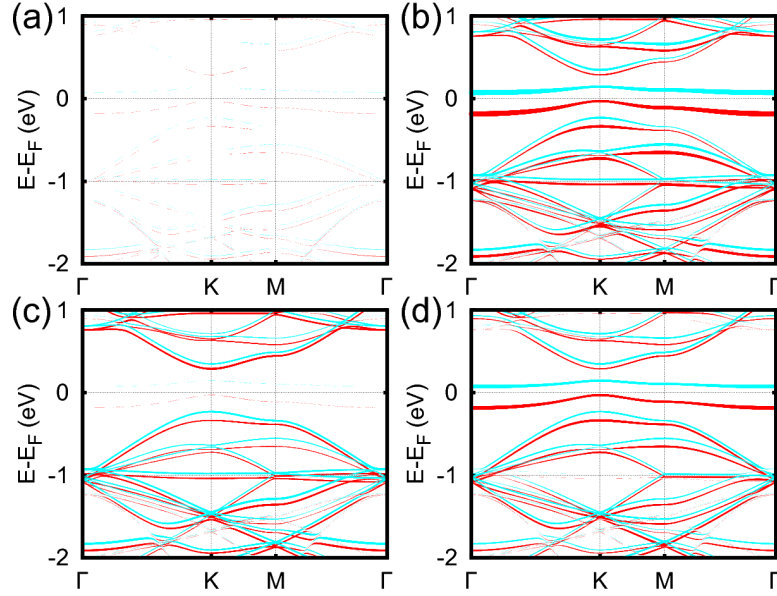


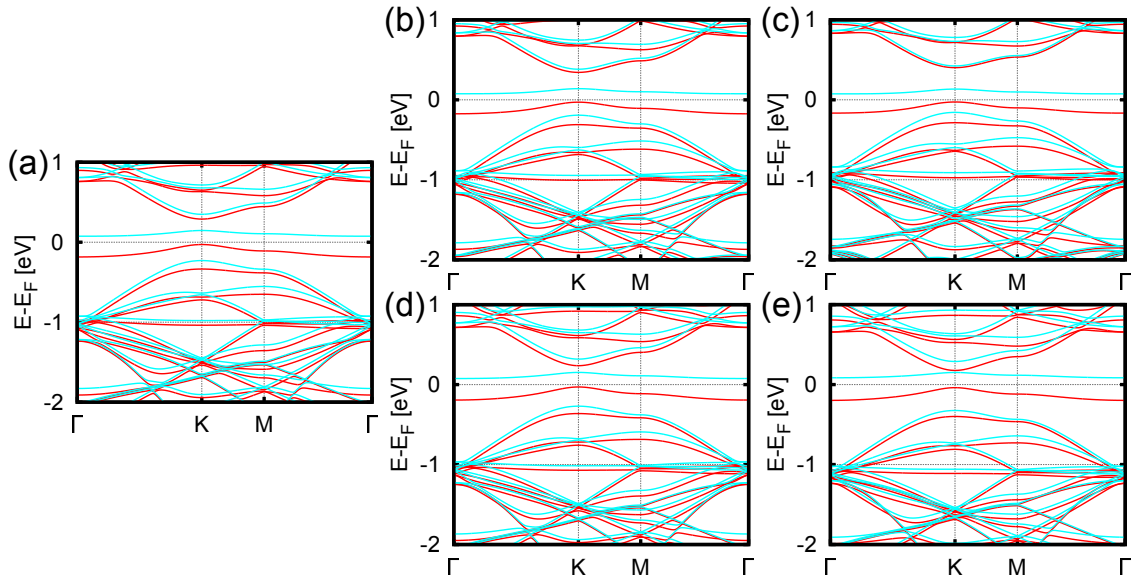
# Supplementary Materials: Tuning the Electronic Structure of Hydrogen-Decorated Silicene

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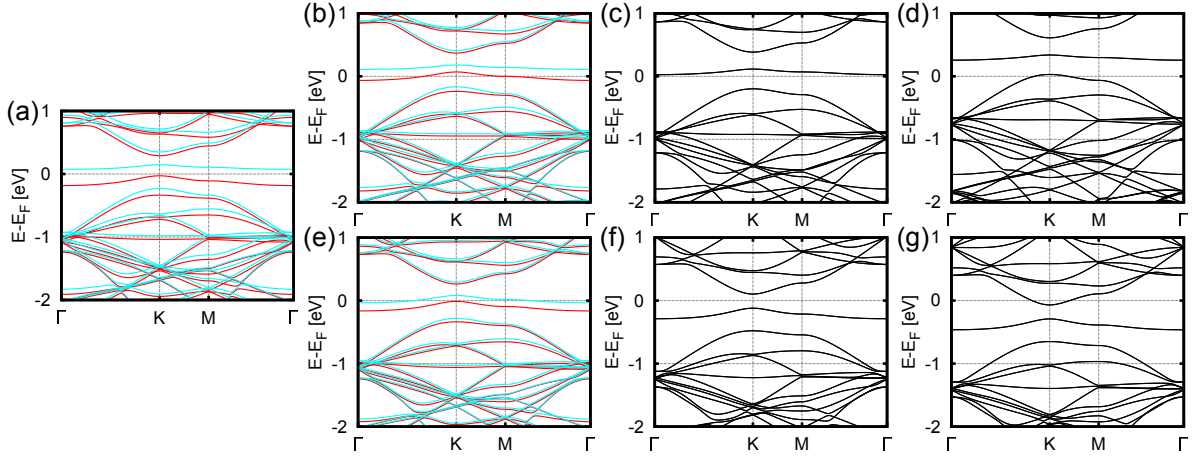
## 1. Band Structure of H/Silicene



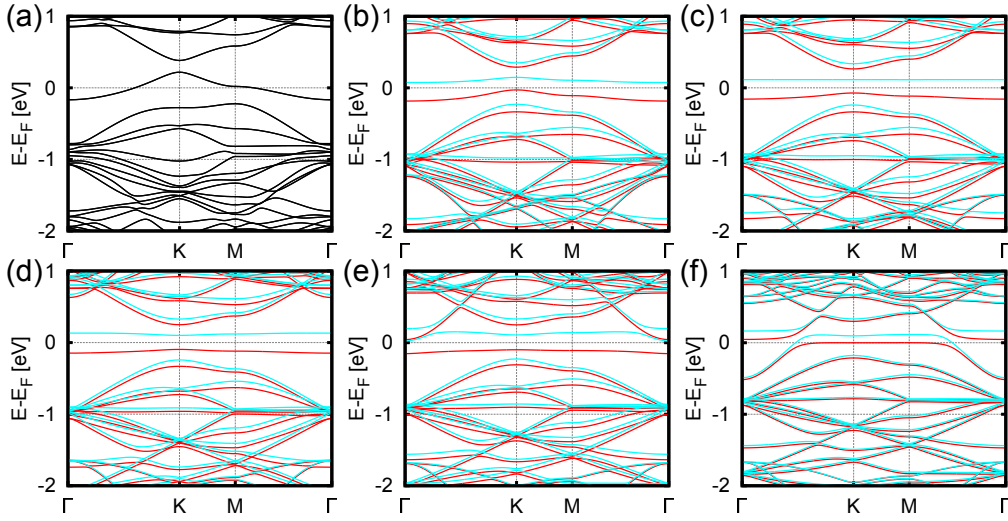
**Figure S1.** The electronic structure of H/silicene system projected on the  $3p_z$  orbitals of different Si atoms,  $\text{Si}_0$ – $\text{Si}_3$  (a)–(d). Red (dark) and cyan (light) symbols indicate the spin-up and spin-down bands, respectively. The thickness of symbols is proportional to the atomic character of bands.



**Figure S2.** The band structure of H/silicene in external electric field. Electric field in panels (a)–(e) are: 0, 0.5, 1,  $-0.5$ , and  $-1$  V/Å. Red (dark) and cyan (light) symbols indicate the spin-up and spin-down bands, respectively.



**Figure S3.** Variations of the band structure for doped system. Panels (a)–(g) represent results for doping: 0.0, 0.025, 0.05, 0.075,  $-0.025$ ,  $-0.0625$ , and  $-0.075$  in units of  $|e|$  per  $1 \times 1$  unit cell. Red (dark) and cyan (light) symbols indicate the spin-up and spin-down bands, while black lines denote the spin-degenerated bands.



**Figure S4.** The band structure of strained H/silicene system. Panels (a)–(f) correspond to the following values of the strain  $\epsilon = -0.025$ , 0, 0.025, 0.05, 0.075, and 0.10. Red (dark) and cyan (light) symbols indicate the spin-up and spin-down bands, while black lines denote the spin-degenerated bands.