Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Tunable band gaps in silicene/MoS_2 heterobilayers

N. Gao, J. C. Li,* Q. Jiang*

Key Laboratory of Automobile Materials (*Jilin University*), *Ministry of Education*, *and School of Materials Science and Engineering*, *Jilin University*, *Changchun*, *130022*, *China*

* Author to whom any correspondence should be addressed: Fax: +86 431 85095876; E-mail: ljc@jlu.edu.cn, jiangq@jlu.edu.cn.

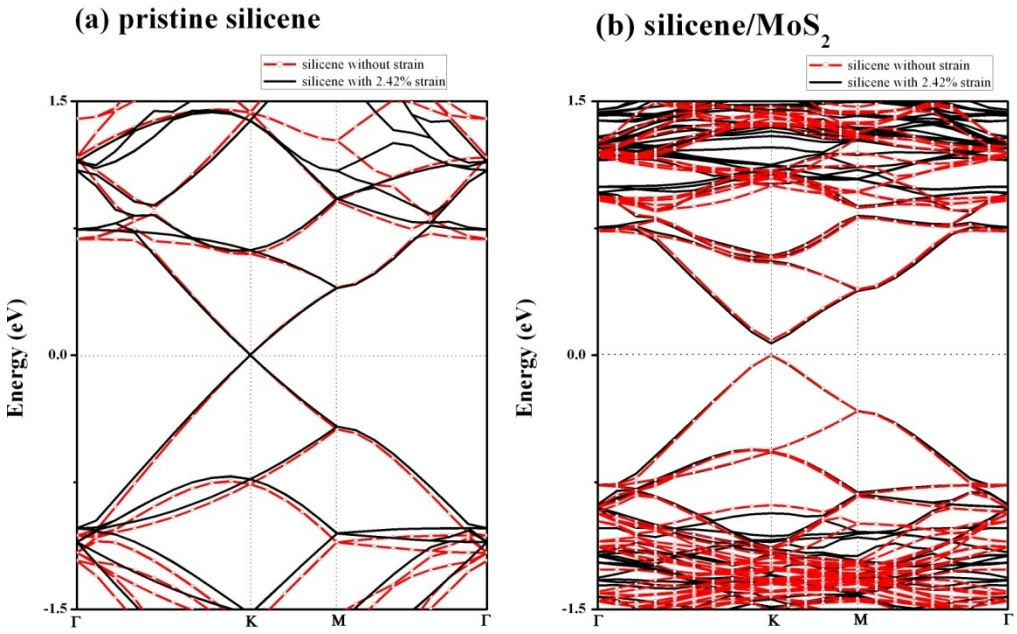

Fig. S1 The band structures of (a) pristine silicene and (b) stable silicene/MoS_2 heterobilayer. The both adopt two matching procedures: silicene without strain and silicene with 2.42% stain.

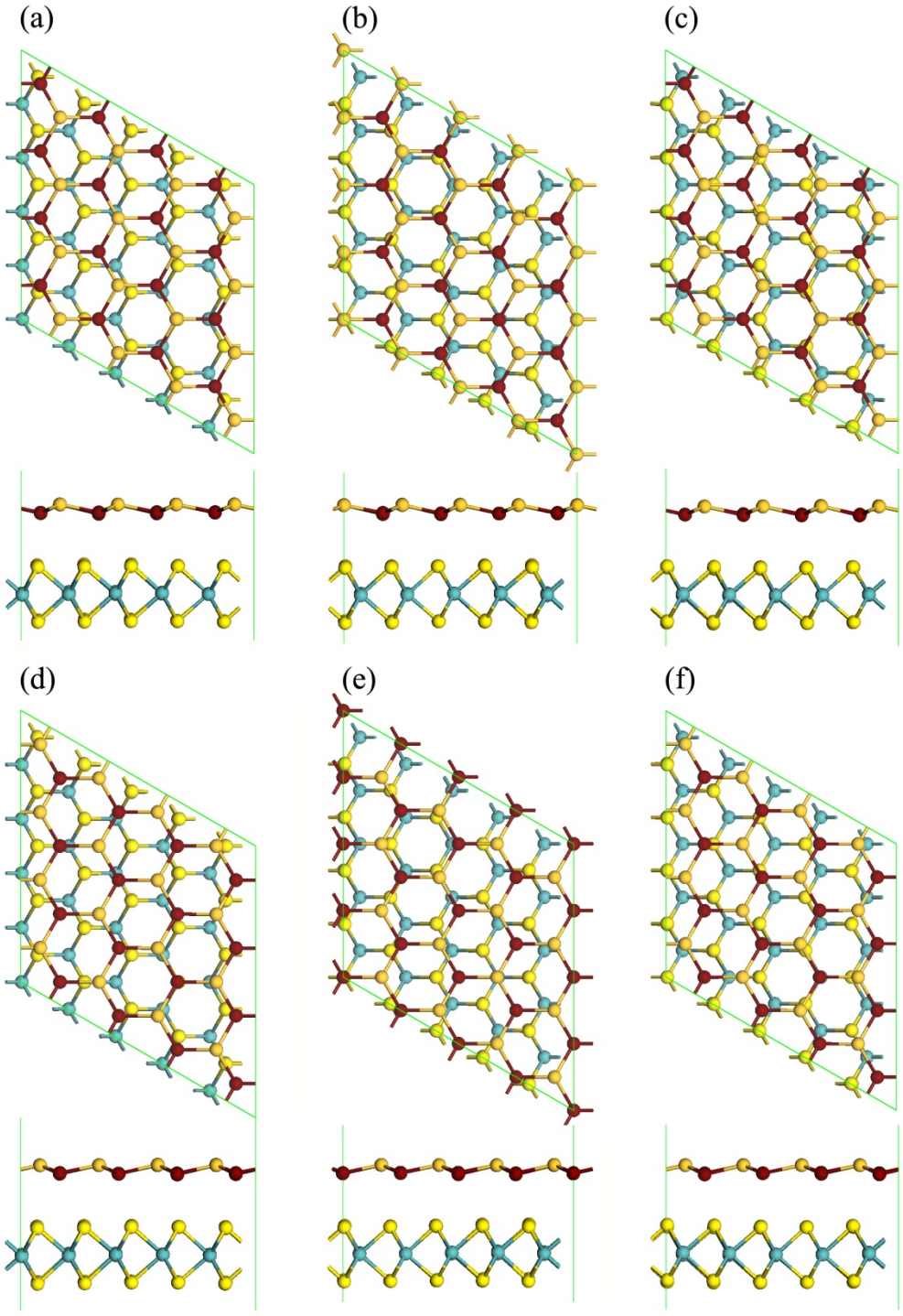

Fig. S2 Top and side views of silicene/MoS_2 configurations. The yellow, blue, khaki and brown balls denote S, Mo, A and B sublattices of Si atoms in silicene, respectively. The supercell is represented by the green lines.

Table S1: Structural parameters and electronic properties of silicene/MoS_2 heterobilayers shown in Fig. S2. E_b (meV/Si), d (Å) and E_g (meV) stand for binding energy, interlayer distance and band gap values, respectively.

Structure	E_b (meV/Si)	d (Å)	E_g (meV)
a	120.32	2.93	70
b	119.32	2.96	52
c	119.53	2.95	51
d	119.88	2.95	50
e	120.04	2.93	71
f	120.04	2.92	72