

## Supplementary material

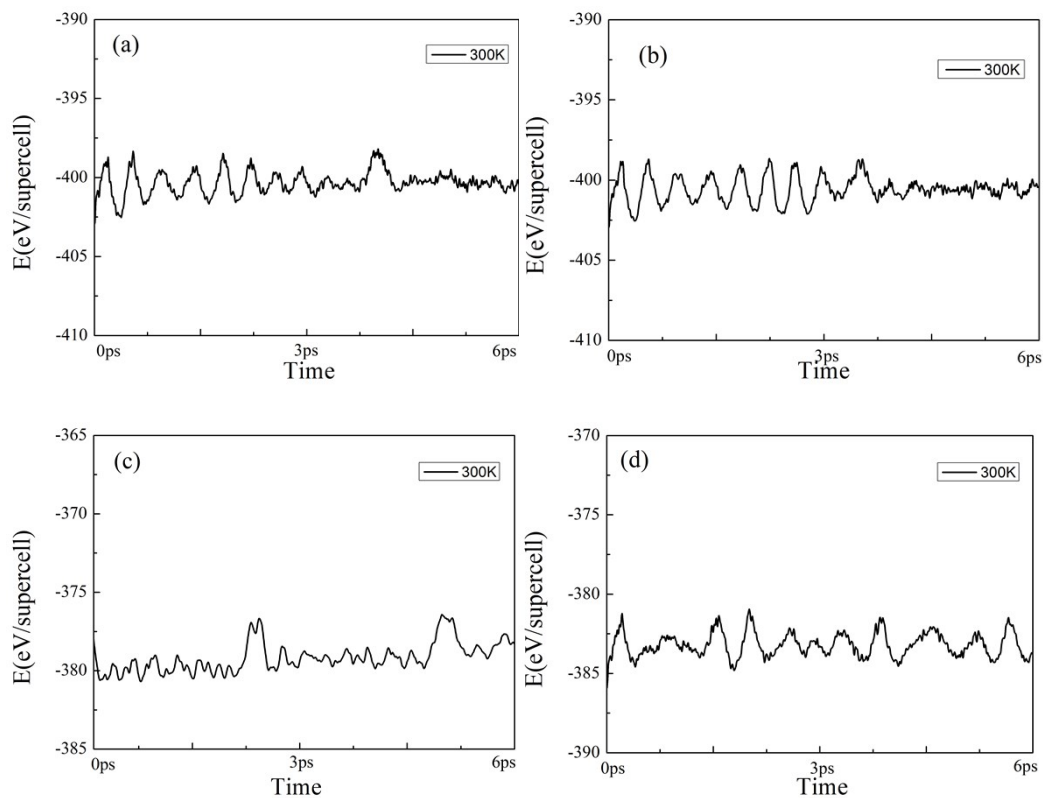
### Modulation of electronic band structure of silicene by polar two-dimensional substrates

Table.S1. the exfoliation energy ( $E_{\text{exf}}$ ) and band gap of Si/Janus

Species	Band gap(eV)	$E_{\text{exf}}(\text{meV}/\text{\AA}^2)$
$\text{Ga}_2\text{SSe}(\text{S}/\text{Se})$	0.1360/0.1680	15/19
$\text{In}_2\text{SSe}(\text{S}/\text{Se})$	0.1437/0.1379	16/16
$\text{GaInS}_2(\text{Ga}/\text{In})$	0.1539/0.1790	15/17

Table.S2. The elastic constants of structure. The unit is N/m

Structure	$C_{11}$	$C_{12}$	$C_{66}$
$\text{Ga}_2\text{SSe}/\text{S}$	133.22	35.79	1.07
$\text{Ga}_2\text{SSe}/\text{Se}$	132.57	35.48	1.25
$\text{In}_2\text{SSe}/\text{S}$	121.93	37.40	1.31
$\text{In}_2\text{SSe}/\text{Se}$	119.57	37.99	2.83
$\text{GaInS}_2/\text{Ga}$	126.46	36.59	1.19
$\text{GaInS}_2/\text{In}$	125.70	36.53	2.11



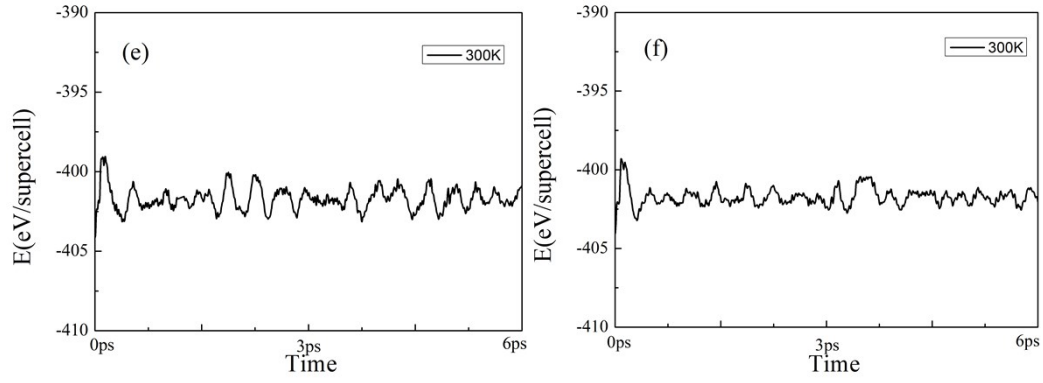


Figure.S1. Energy fluctuations of (a) Si/Ga<sub>2</sub>SSe-S, (b) Si/Ga<sub>2</sub>SSe-Se, (c) Si/In<sub>2</sub>SSe-S, (d) Si/In<sub>2</sub>SSe-Se, (e) Si/GaInS<sub>2</sub>-Ga, (f) Si/GaInS<sub>2</sub>-In during MD simulations at 300K.

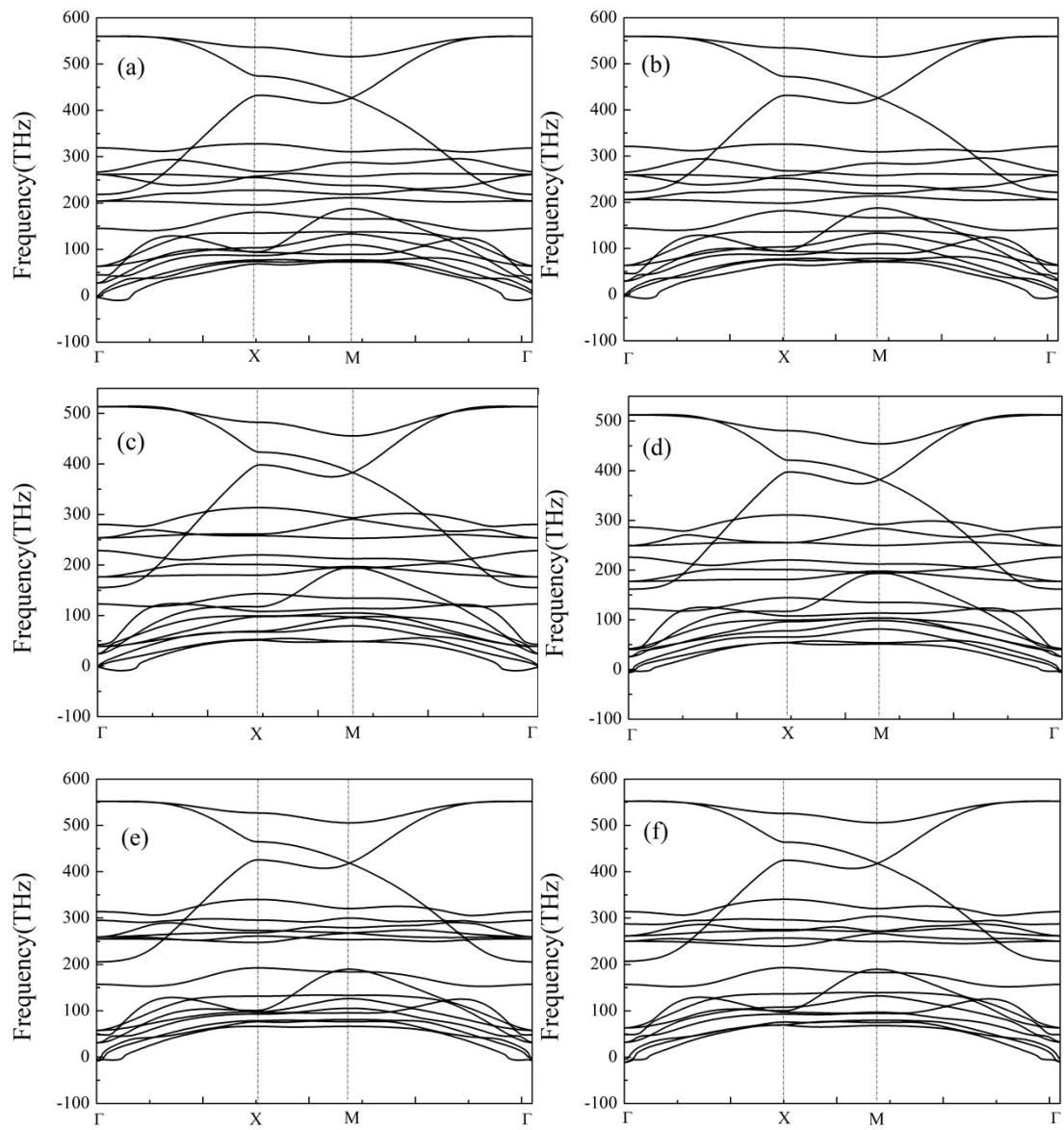


Figure.S2. Phonon spectrum of (a) Si/Ga<sub>2</sub>SSe-S, (b) Si/Ga<sub>2</sub>SSe-Se, (c) Si/In<sub>2</sub>SSe-S, (d) Si/In<sub>2</sub>SSe-Se, (e) Si/GaInS<sub>2</sub>-Ga, (f) Si/GaInS<sub>2</sub>-In.

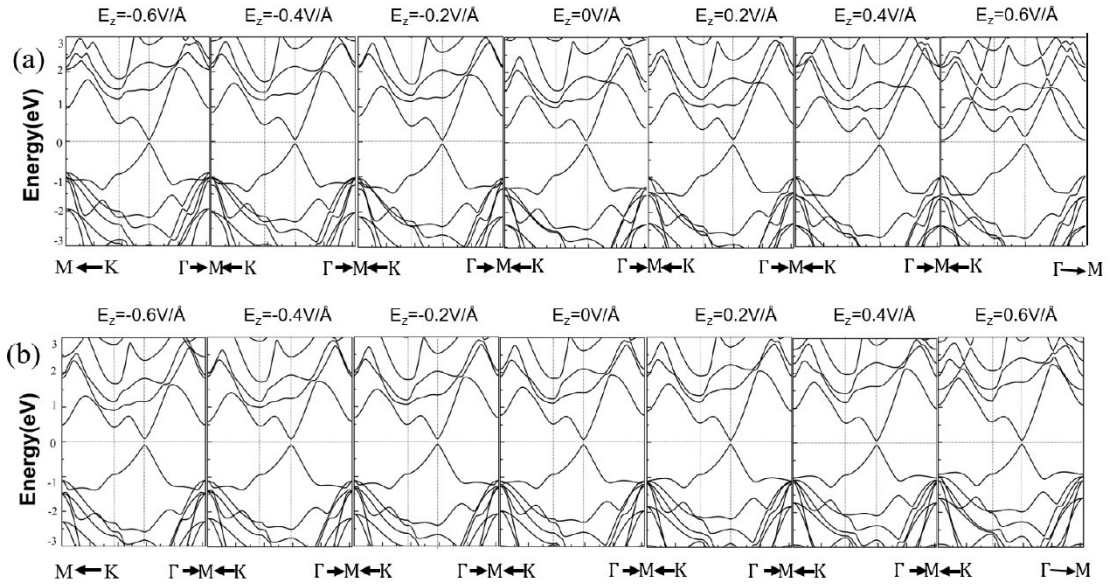


Figure.S3. Band structures near the Fermi levels of (a) the Si/In<sub>2</sub>SSe heterojunction with Si/S interface and (b) the Si/In<sub>2</sub>SSe heterojunction with Si/Se interface under different electric fields  $E_z$

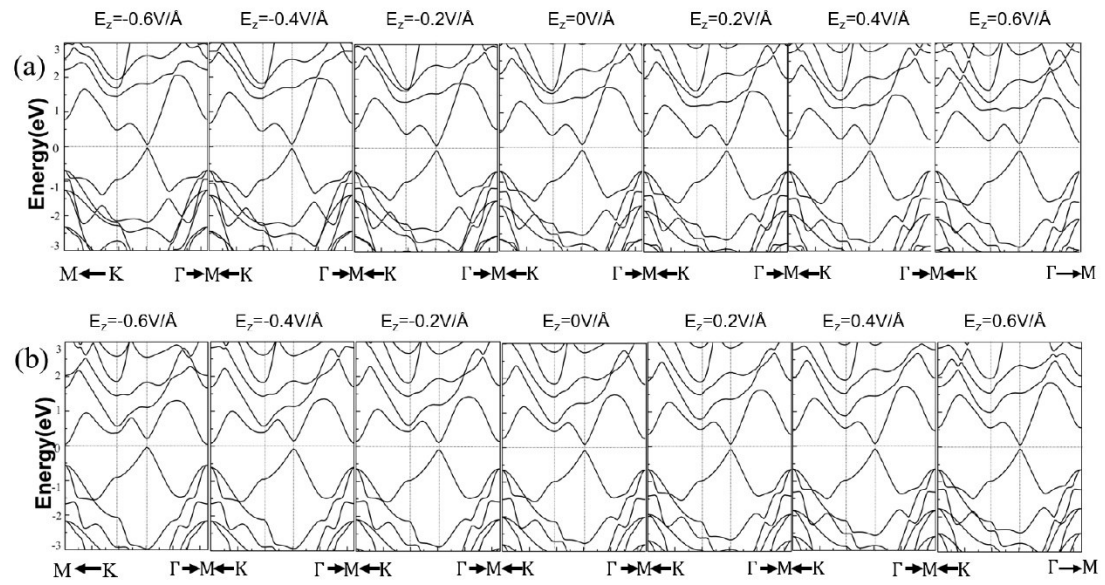


Figure.S4. Band structures near the Fermi levels of (a) the Si/GaInS<sub>2</sub> heterojunction with Si/Ga interface and (b) the Si/GaInS<sub>2</sub> heterojunction with Si/In interface under different electric fields  $E_z$ .