Supplementary Material

An analysis of Schottky barrier in silicene/Ga_2SeS heterostructures by employing electric field and strain

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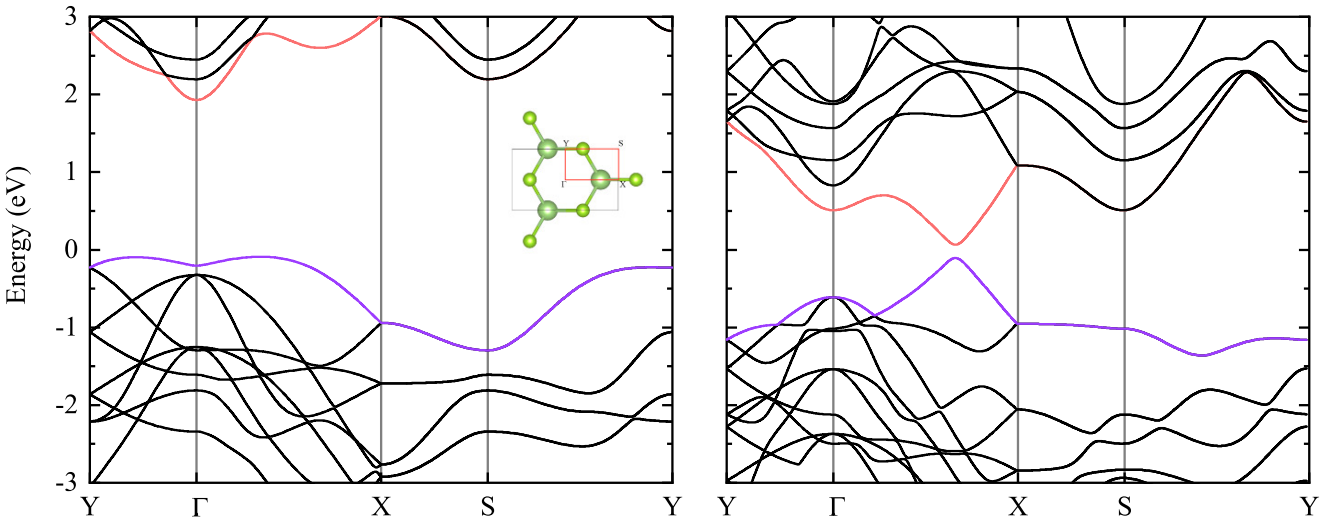

FIG. S1: The electronic band structures of orthogonal Ga_2SeS and silicene/Ga_2SeS heterostructure.

Pseudo-atomic localized basis function had been performed by using OpenMX 3.9 package [1] for first principles calculations. The Perdew-Burke-Ernzerhof approach from the generalized gradient approximation (PBE-GGA) [2] was applied to describe the exchange-correlation functional and the norm conserving pseudopotentials [3–5]. The Brillouin zone integration was performed with $17 \times 17 \times 1$ k-point mesh using the Monkhrost-Pack method [6]. The energy cutoff was set to be 300 Ry. A vacuum space of 25 Å was applied in the direction perpendicular to the sheet to avoid the interaction between imaginary images. Geometry optimization was performed until the maximum force on each atom was less than 0.002 Hartree/Bohr.

References

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[2] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
[3] T. Ozaki, Phys. Rev. B **67**, 155108 (2003).
[4] T. Ozaki and H. Kino, Phys. Rev. B **69**, 195113 (2004).
[5] T. Ozaki and H. Kino, Phys. Rev. B **72**, 045121 (2005).
[6] H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976).

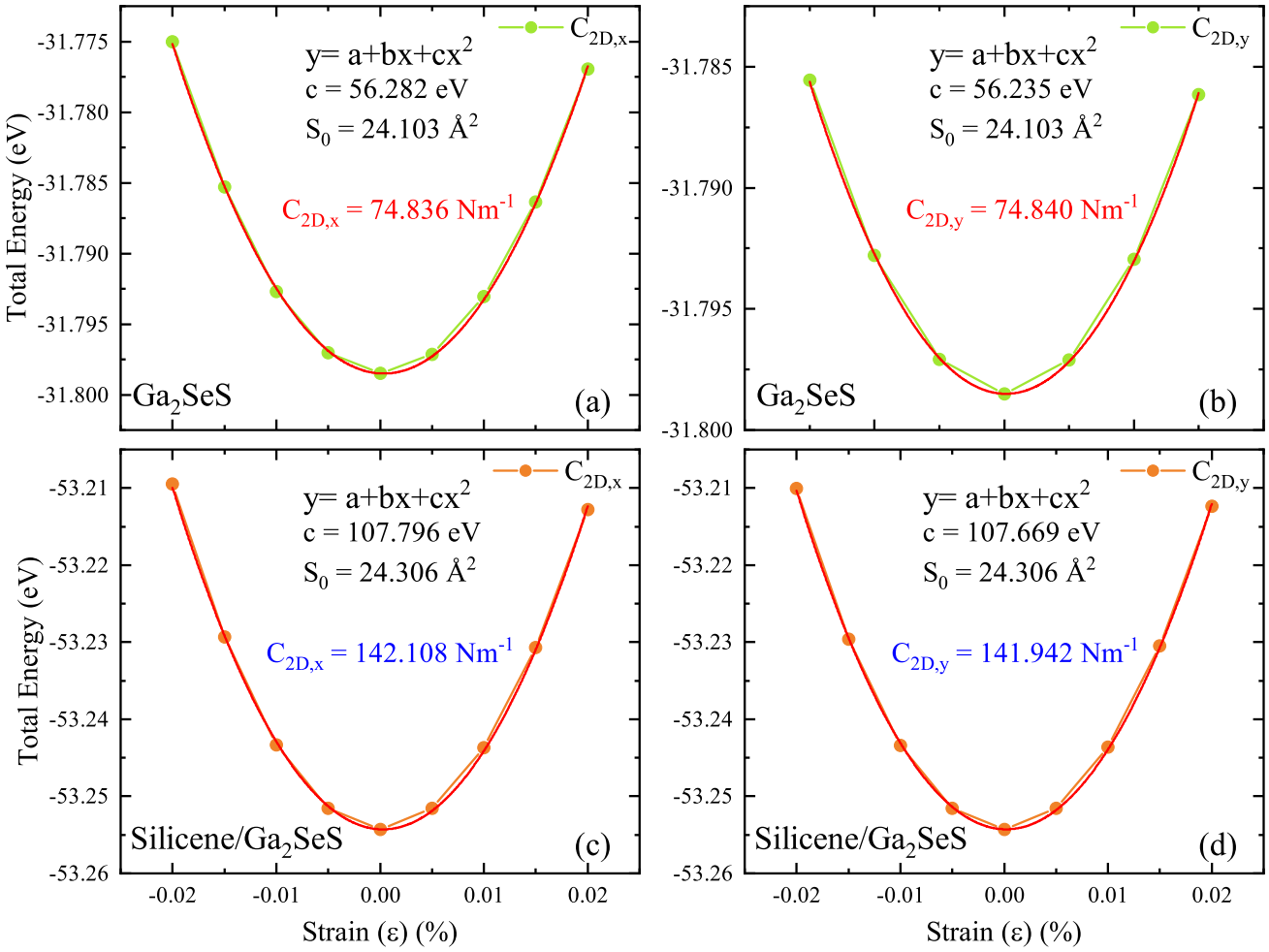

FIG. S2: The variation of total energies of monolayer Ga_2SeS and silicene/Ga_2SeS heterostructure under the presence of uniaxial strain.

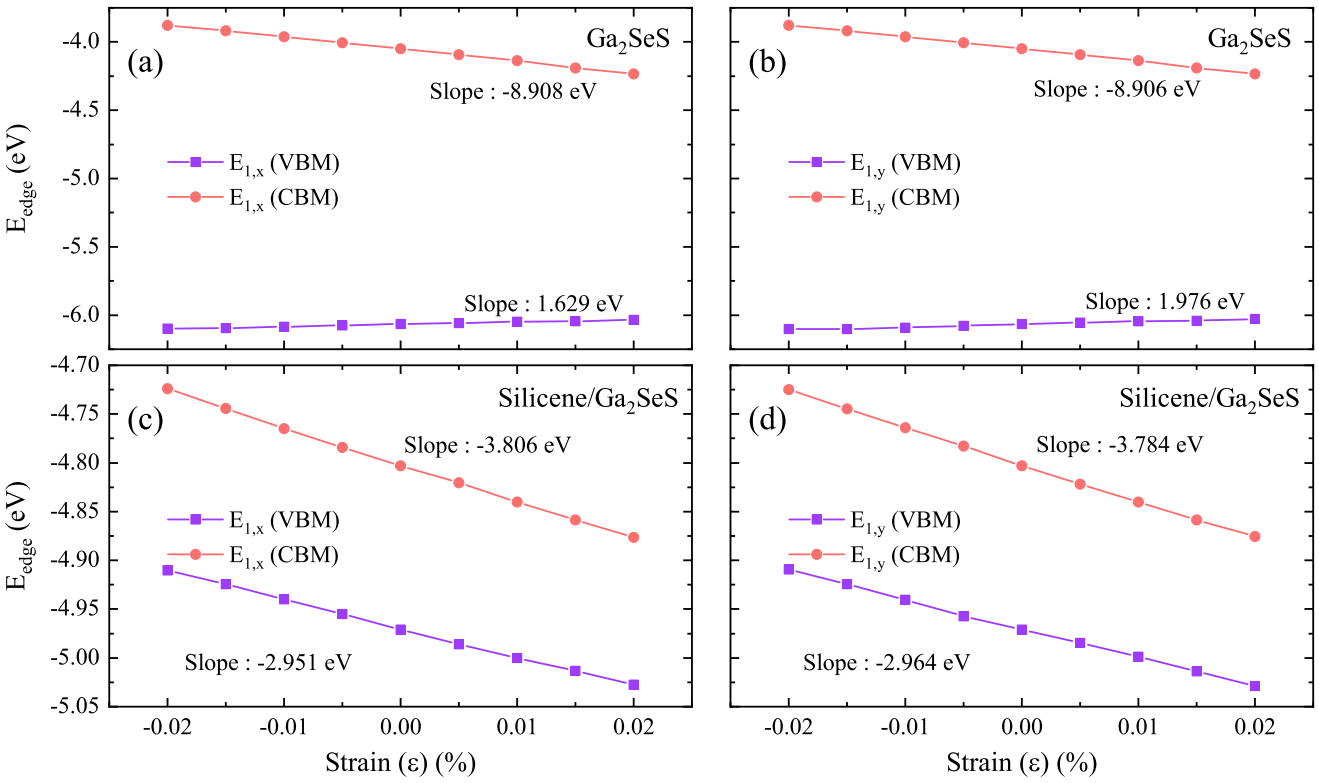

FIG. S3: Band edge positions of (a)-(b) monolayer Ga_2SeS and (c)-(d) silicene/Ga_2SeS heterostructure as a function of uniaxial strain in x and y directions.

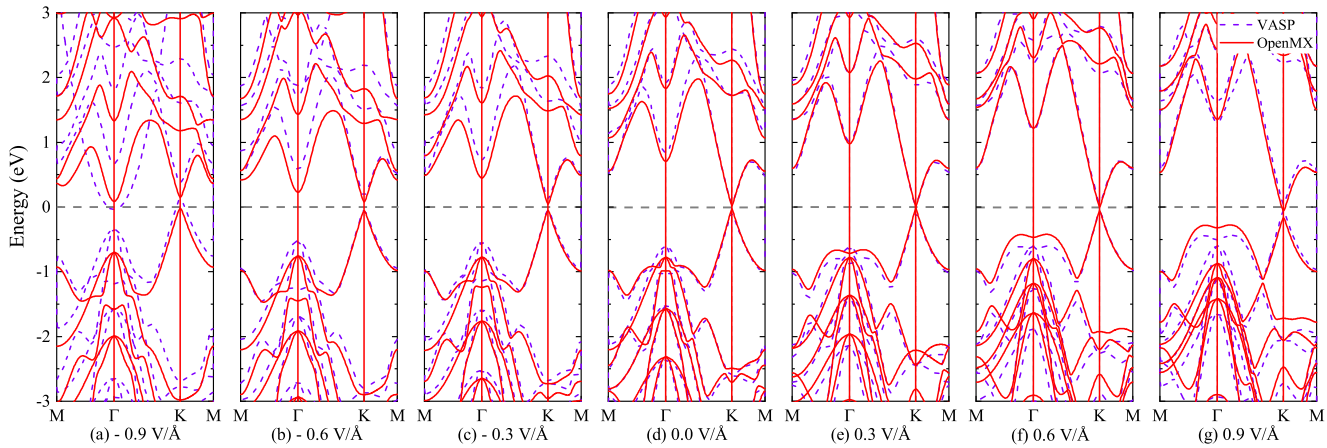

FIG. S4: The electronic band spectrum of the variation of perpendicular electric field.