Supporting Information

The electronic and magnetic properties modulated by ferroelectric polarization switching in two-dimensional VSeTe/Sc_2CO_2 van der Waals heterostructure

Weiyang Yu,[1,*] Xiaoli Zhang,[1] Yuling Zhang,[1] Yali Wu,[1] Rui Li,[1] Wei-Bing Zhang[2, †]

[1] School of Physics and Electronic Information Engineering, Henan Polytechnic University, Jiaozuo, 454000, Henan, China

[2] Hunan Provincial Key Laboratory of Flexible Electronic Materials Genome Engineering, Changsha University of Science and Technology, Changsha, 410114, Hunan, China

Corresponding authors: [*]yuweiyang@hpu.edu.cn; [†]zhangwb@csust.edu.cn

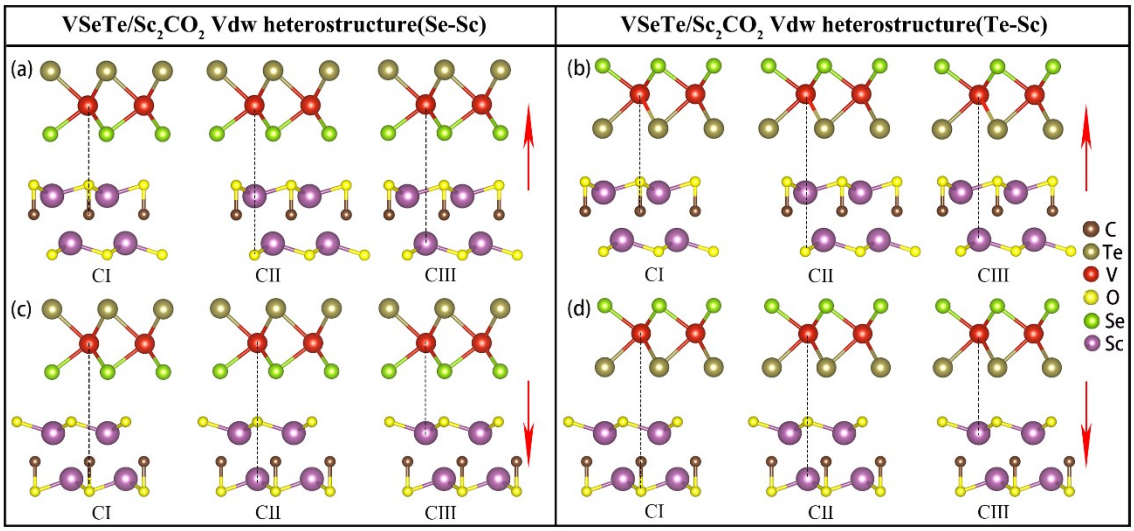

Fig. S1 12 kinds of heterogeneous structural types. Among them, (a) and (b) are three highly symmetric configurations with ferroelectric polarization upward of Se-Sc and Te-Sc as the contact surface; (c) and (d) are three highly symmetrical configurations with ferroelectric polarization downward of Se-Sc and Te-Sc as the contact surface.

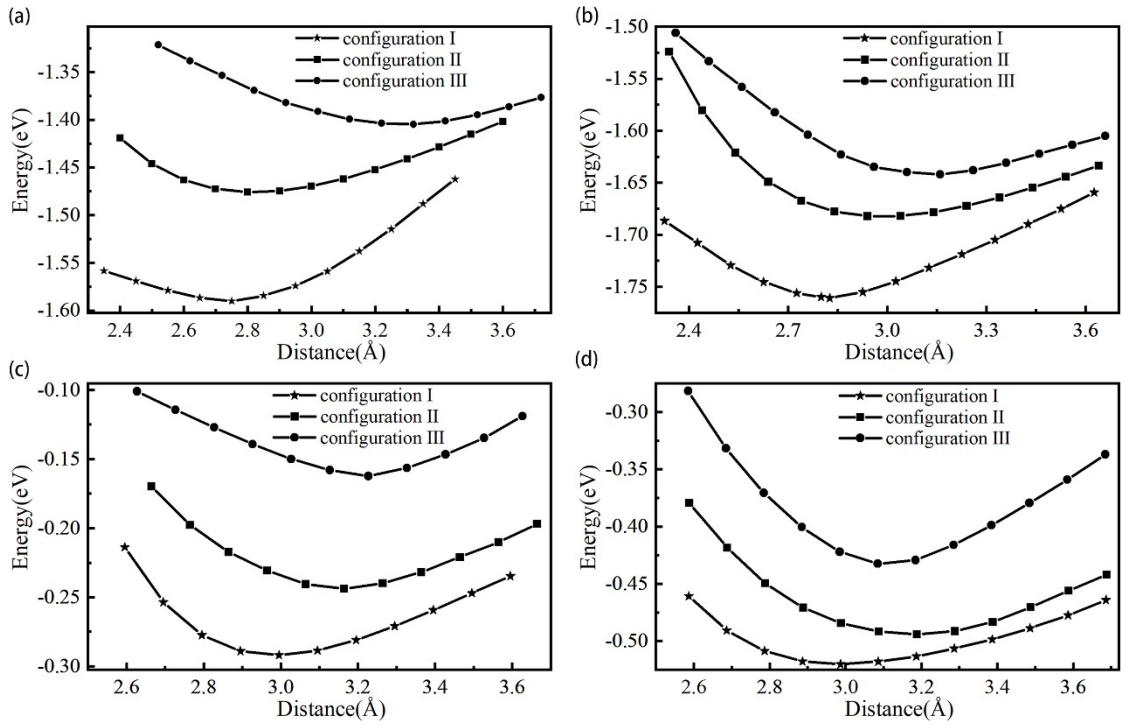

Fig. S2 Relationship between layer spacing and energy of 12 kinds of configurations.Where (a) and (b) are ferroelectric polarization upward and downward heterostructure with Se-Sc as contact surface, respectively. (c) and (d) represent the upward and downward heterostructure

of ferroelectric polarization with Te-Sc as the contact surface, respectively. Star, square and round dots represent CI, CII and CIII configurations, respectively.

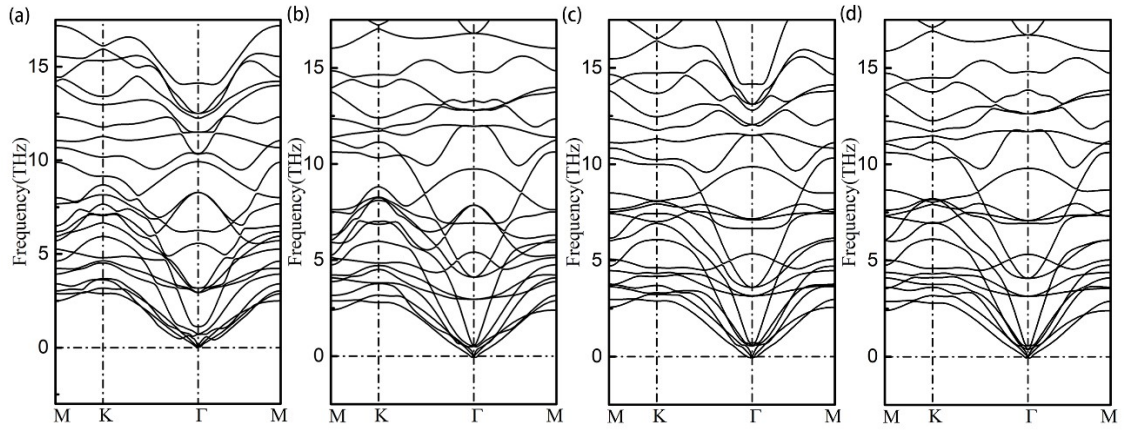

Fig. S3 Phonon spectra corresponding to the four lowest energy configurations: (a) $VSeTe/Sc_2CO_2$ (Se-Sc↑), (b) $VSeTe/Sc_2CO_2$ (Se-Sc↓), (c) $VSeTe/Sc_2CO_2$ (Te-Sc↑), (d) $VSeTe/Sc_2CO_2$ (Te-Sc↓).

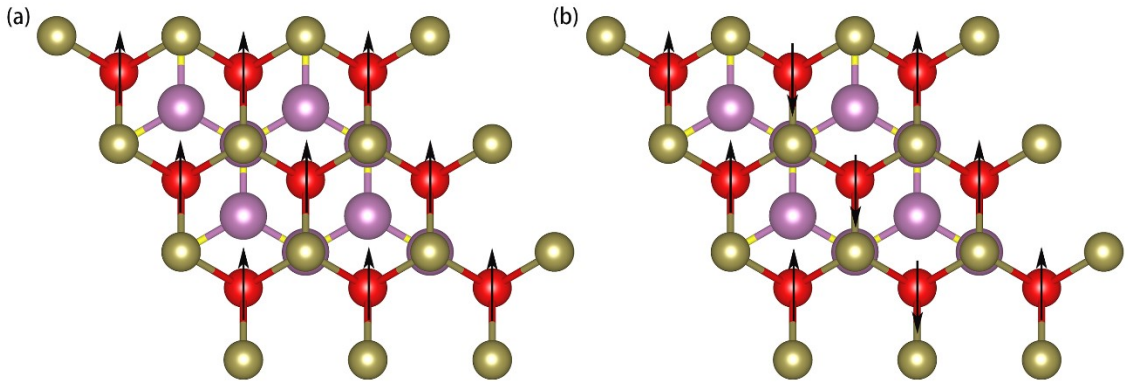

Fig. S4 Ferromagnetic configurations of $VSeTe/Sc_2CO_2$ (Se-Sc↑) heterostructure with (a) ferromagnetic and (b) antiferromagnetic configuration.

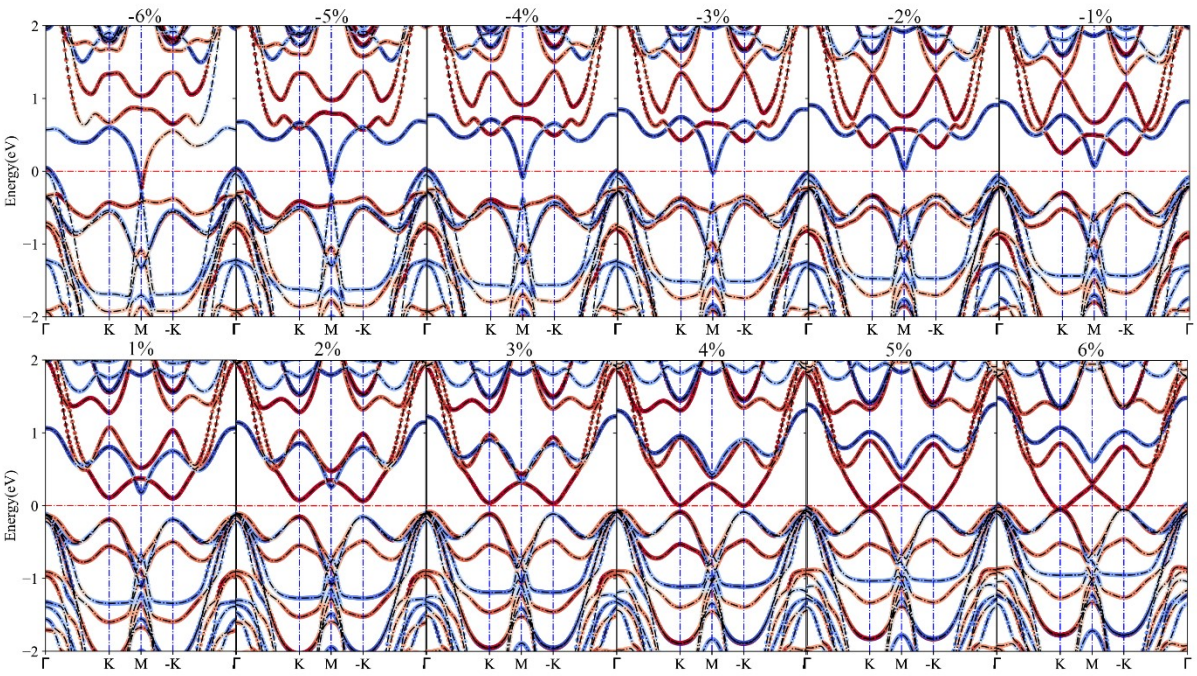

Fig. S5 Band structures of $VSeTe/Sc_2CO_2$ (Se-Sc↓) heterostructures regulated by strain.

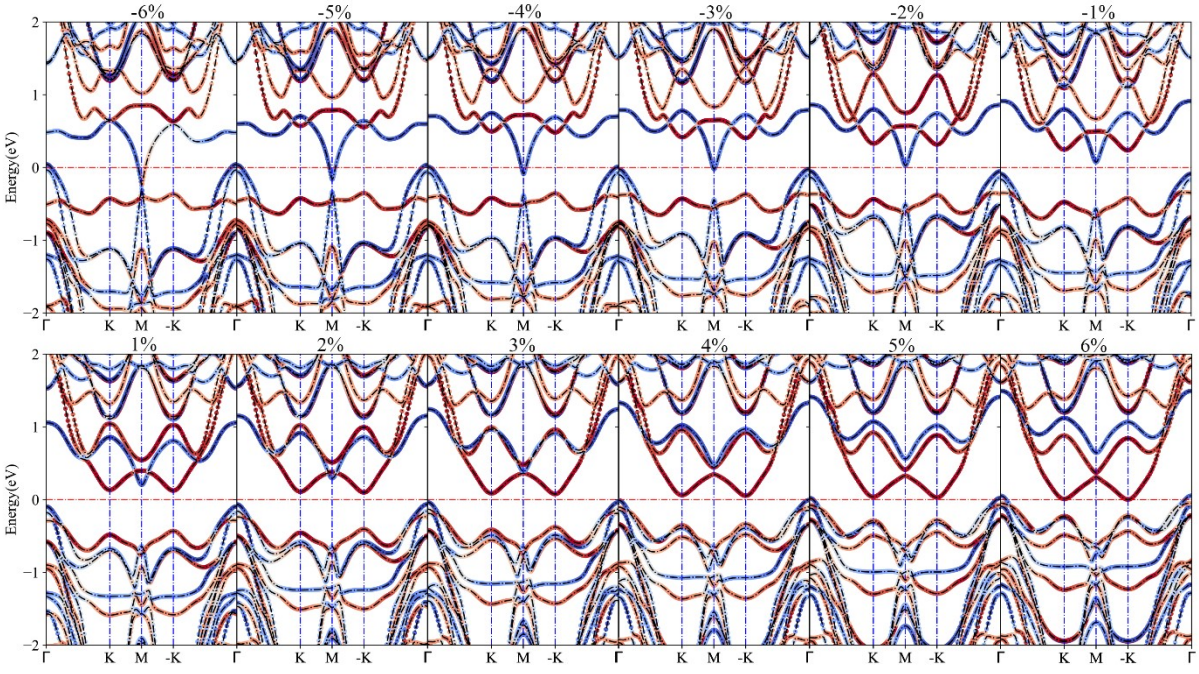

Fig. S6 Band structures of $VSeTe/Sc_2CO_2$ (Te-Sc↓) heterostructures regulated by strain.