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

Supplemental Information

Strain-induced ferroelectric polarization reversal without undergoing geometric inversion in blue SiSe monolayer

Yan-Dong Guo,[1,2,*] Rui-Jie Meng,[1] Xue-Qin Hu,[1] Li-Yan Lin,[1] Yu-Rong Yang,[1,2,*] Ming-Yu Yang,[1] Yun You,[1] Lan-Qi Zhang,[1] Yi-Long Xu, [1] and Xiao-Hong Yan[1,2,3,]

[1]*College of Electronic and Optical Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210046, China*

[2]*Key Laboratory of Radio Frequency and Micro-Nano Electronics of Jiangsu Province, Nanjing 210023, China*

[3]*College of Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China*

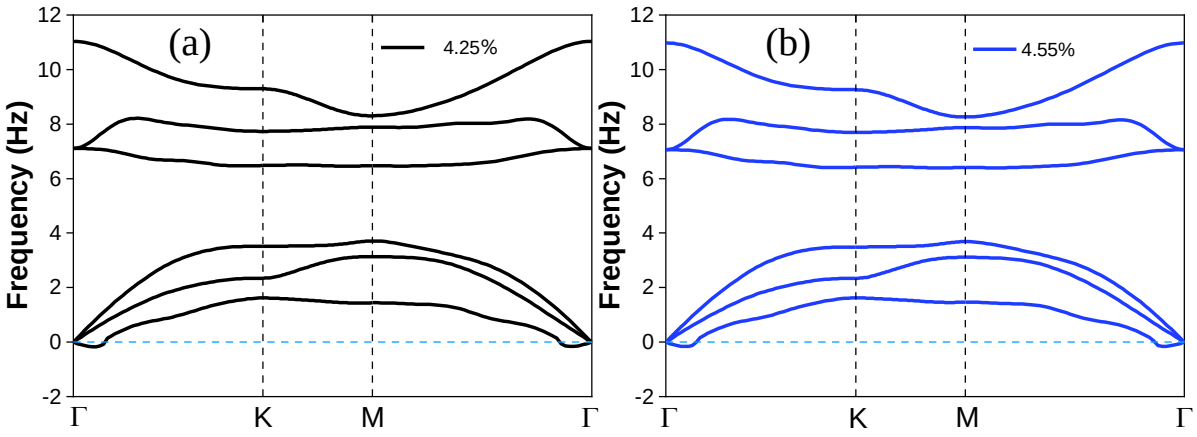

Fig. S1 (a)-(b) The phonon spectra of blue SiSe monolayer under the biaxial in-plane strains of ε=4.25% and 4.55%, respectively.

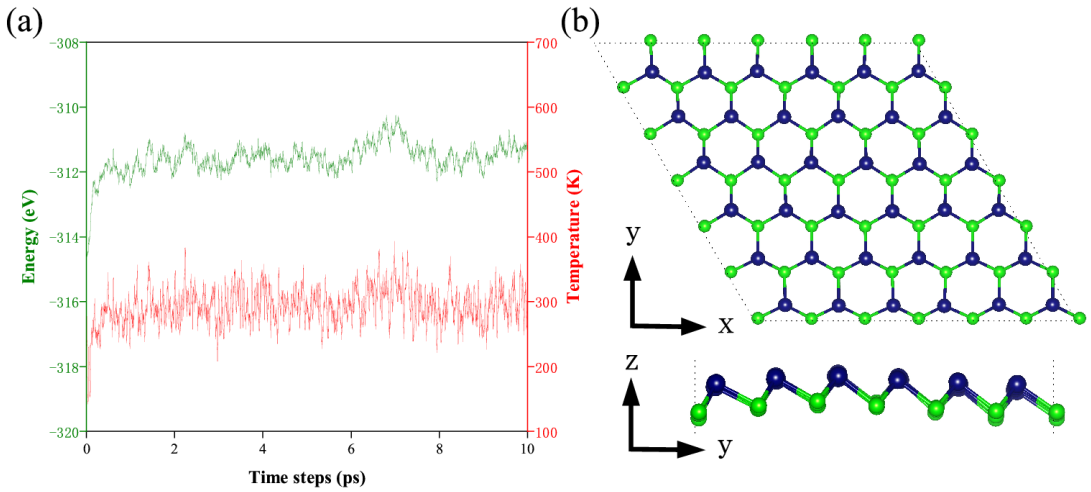

Fig. S2 (a) Energy and temperature fluctuations, (d) Top and side views of monolayer SiSe for AIMD simulations in NpT ensemble. The structure is obtained by averaging the geometries in the last 9000 steps.

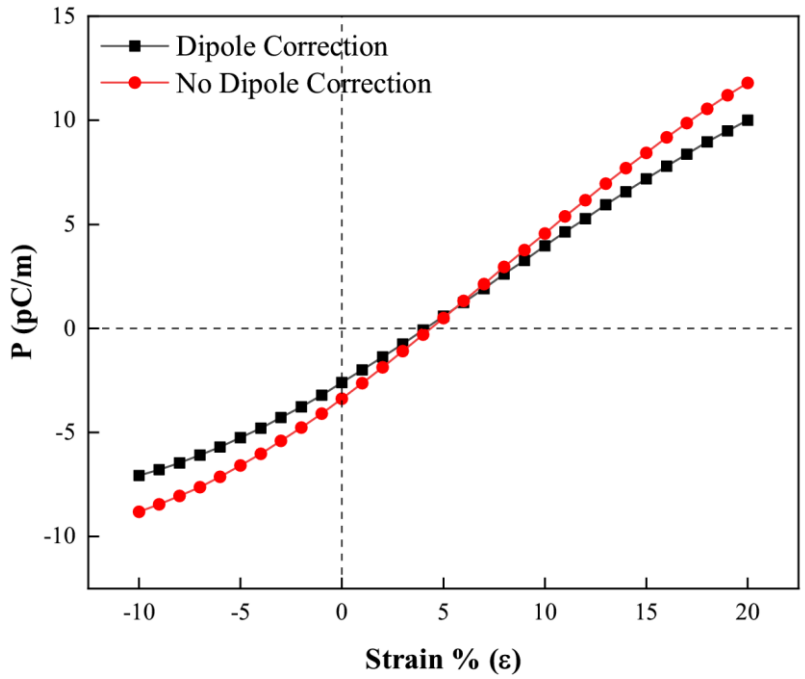

Fig. S3 The ferroelectric polarizations of blue monolayer SiSe vary with the biaxial strain with and without the dipole correction.

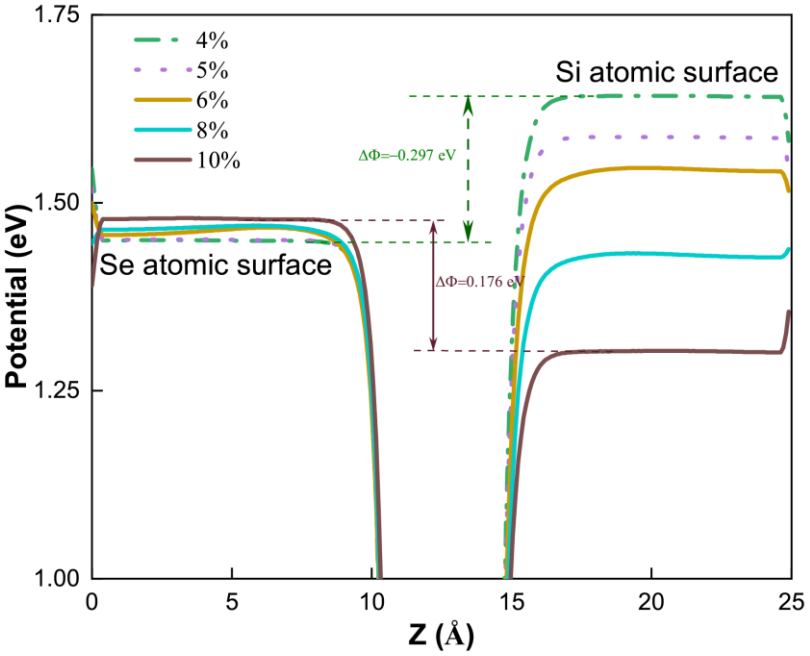

Fig. S4 The average planar potential of blue monolayer SiSe under a biaxial strain.

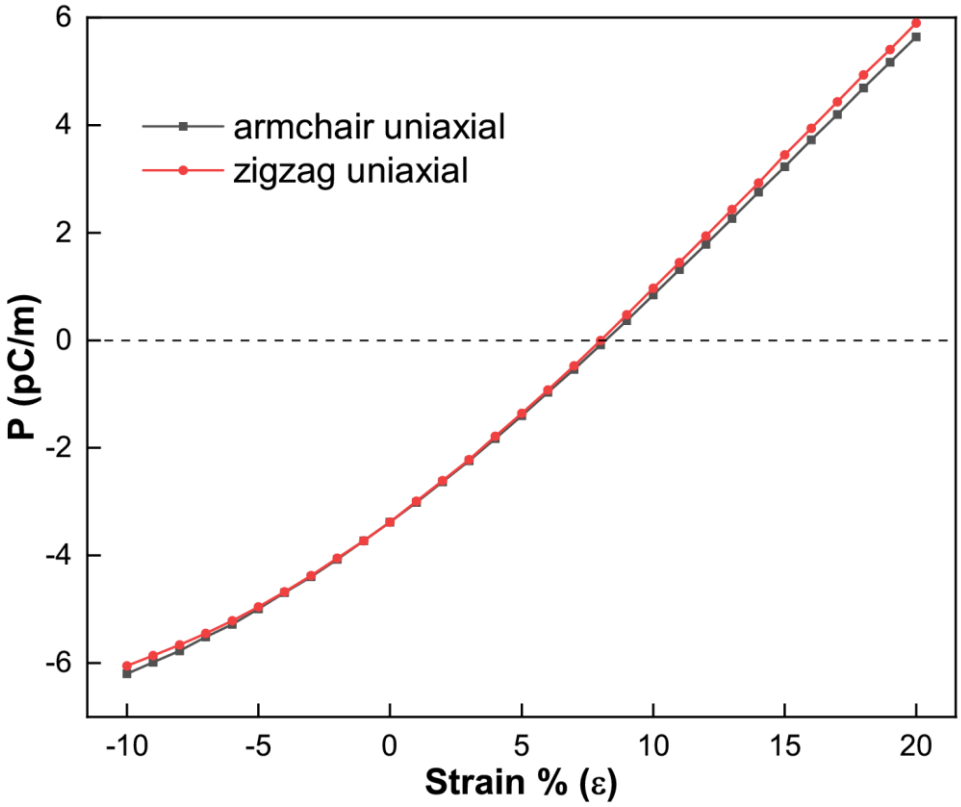

Fig. S5 The polarization varies with the uniaxial strain of ε along armchair and zigzag directions in blue monolayer SiSe.