Supplementary Information (SI) for Journal of Materials Chemistry C.

Strain-tuning of perpendicular magnetic anisotropy and valley topological phase transition in SVNH monolayer

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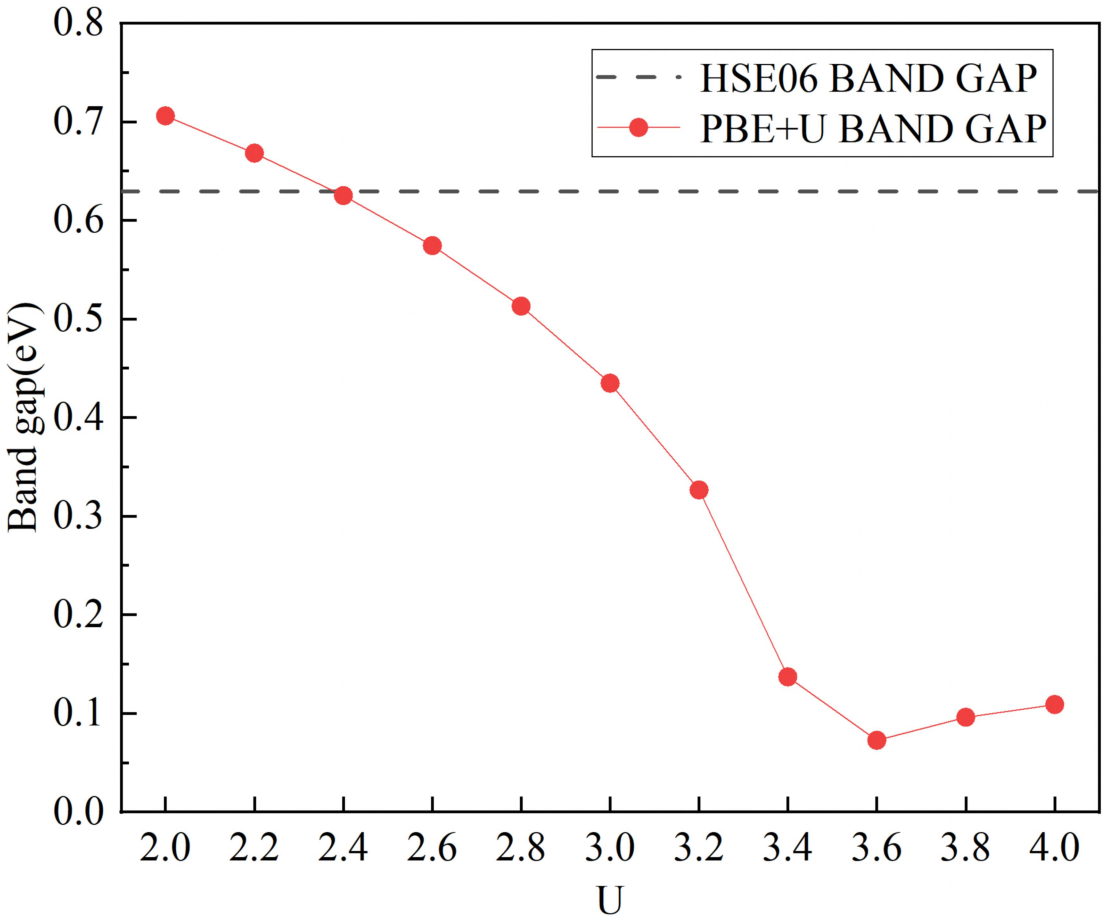

Fig. S1 Comparison of energy band gaps at different U_{eff} values compared to HSE06 energy band gaps.

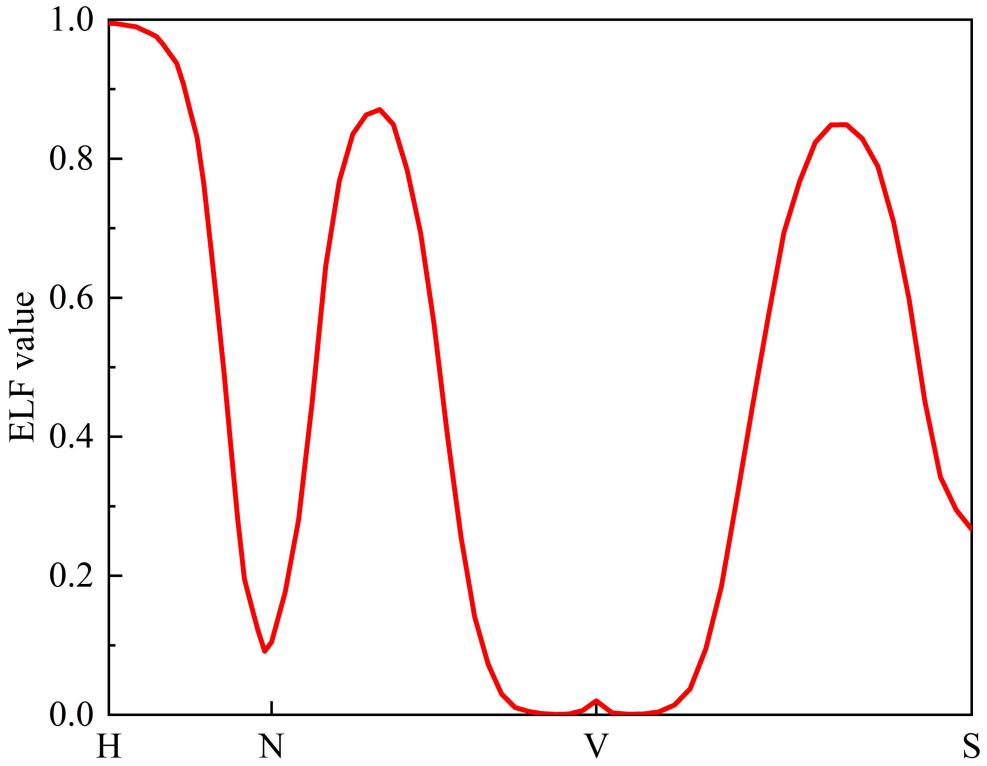

Fig. S2 Electron localization function (ELF) of SVNH monolayer.

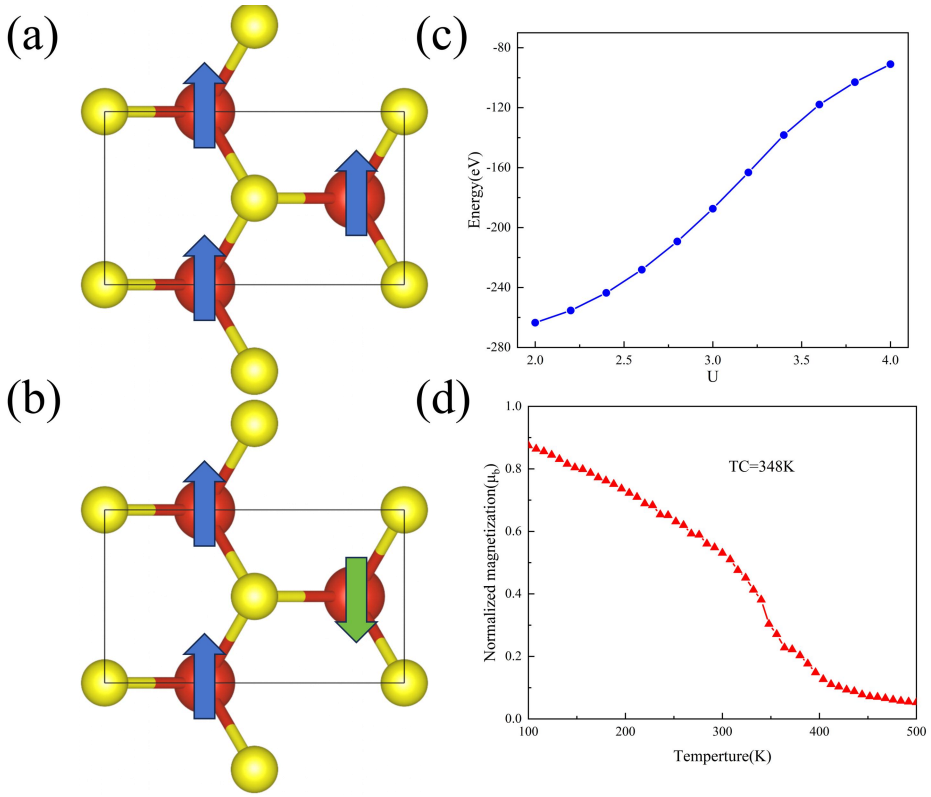

Fig. S3 (a) The FM and (b) AFM configurations of the monolayer SVNH, (c) the energy difference between FM and AFM under different U_{eff}, and (d) the curie-temperature from Monte Carlo simulations.

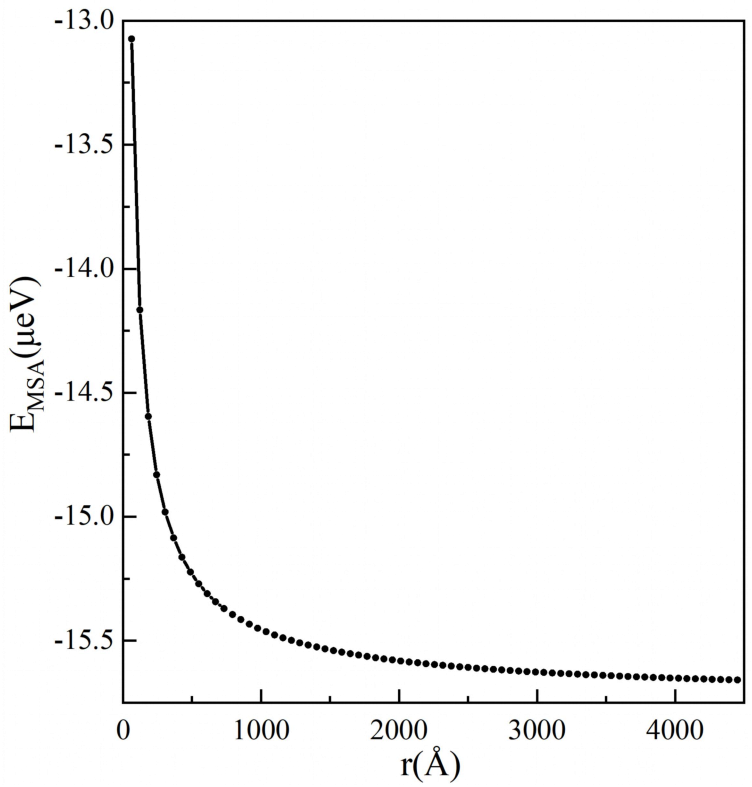

Fig. S4 The relationship between E_{MSA} and the maximum spacing between magnetic atoms

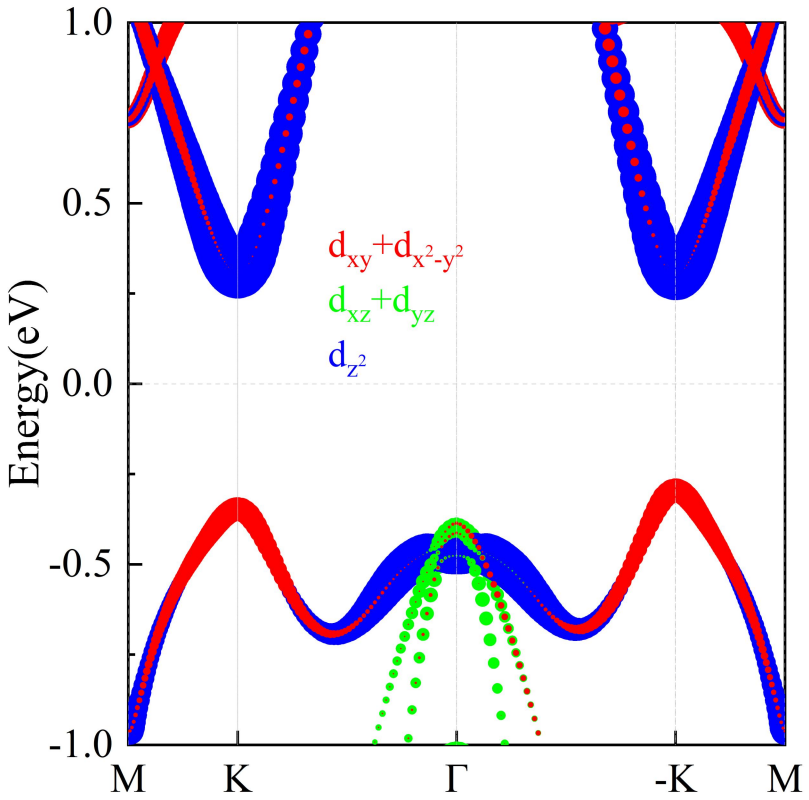

Fig. S5 Projection band diagram of the d-orbitals of V atoms with GGA+U+SOC. The Fermi level set to 0.

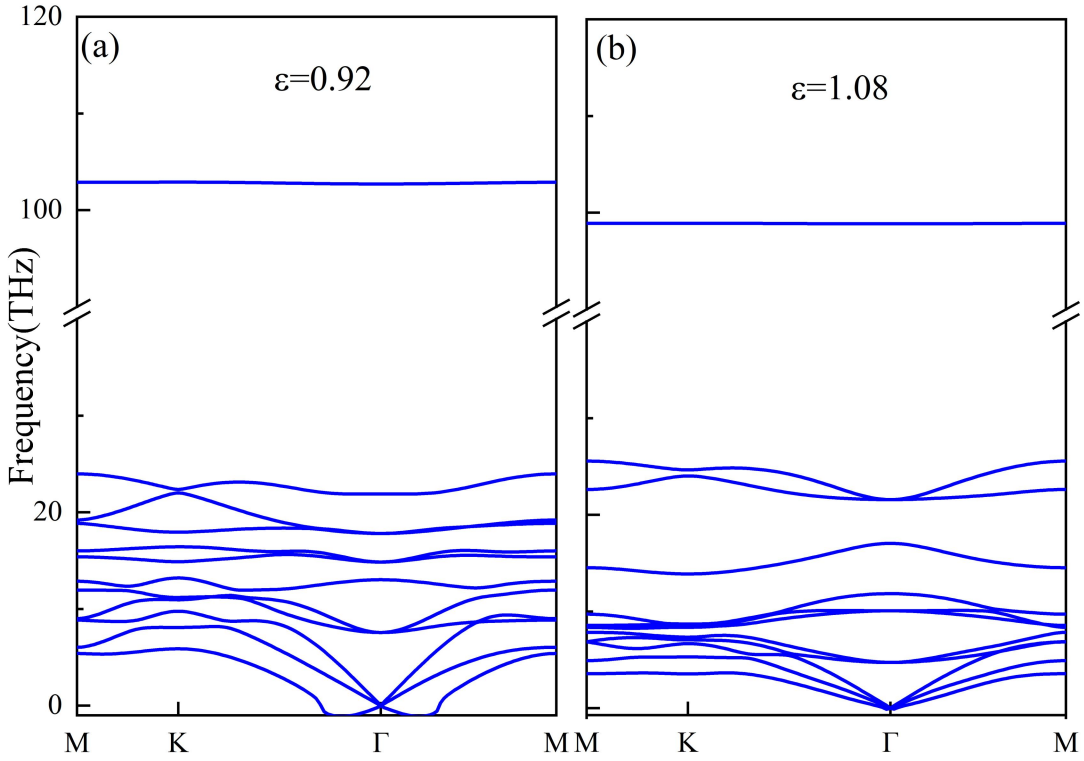

Fig. S6 Phonon spectrum for (a) ε=0.92 and (b) ε=1.08.

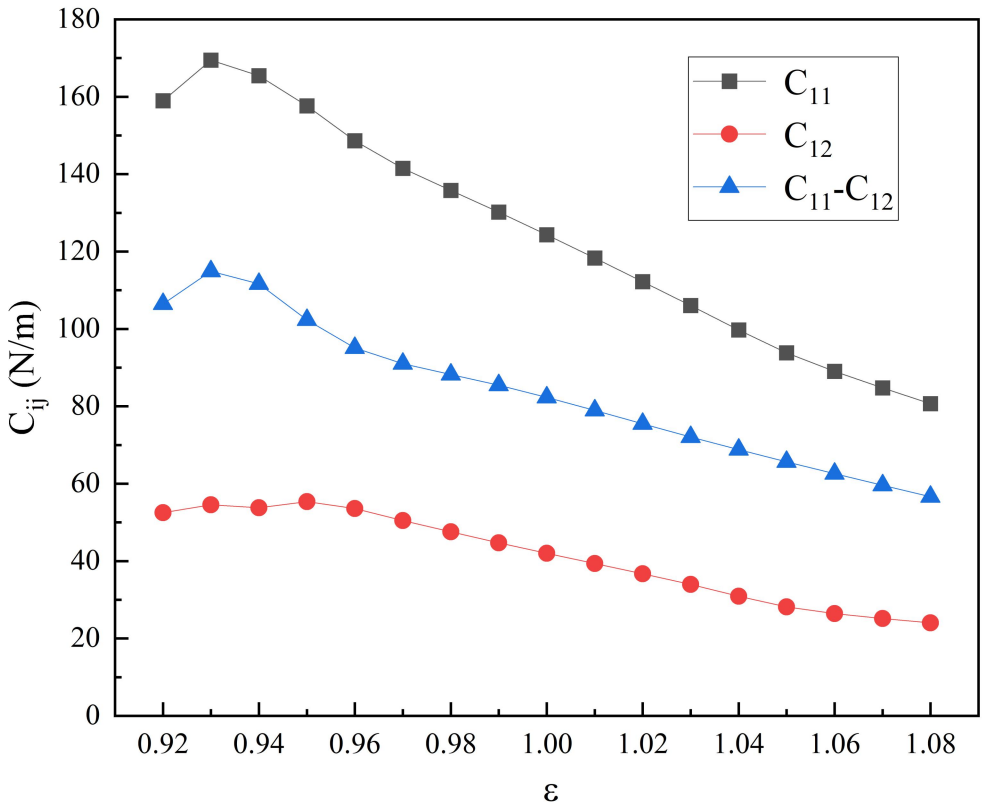

Fig. S7 The elastic constants under different strains, with C_{11} represented in black, C_{12} in red, and C_{11}-C_{12} in blue.

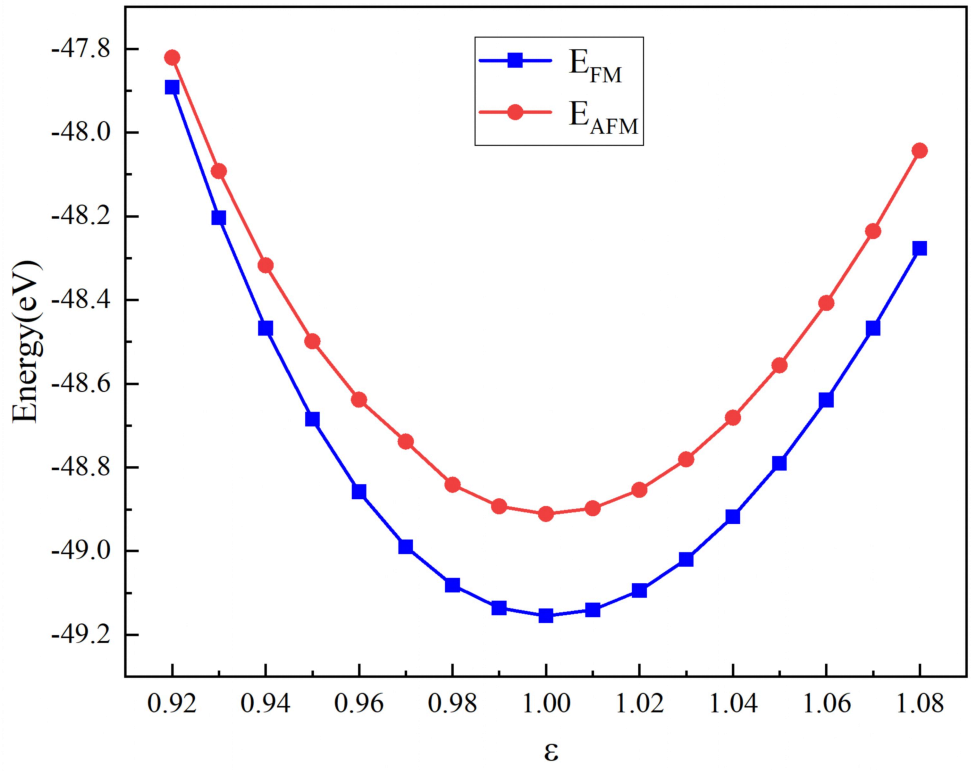

Fig. S8 The E_{FM} and E_{AFM} under different bixial strain. Red represents E_{AFM}, and blue represents E_{FM}.

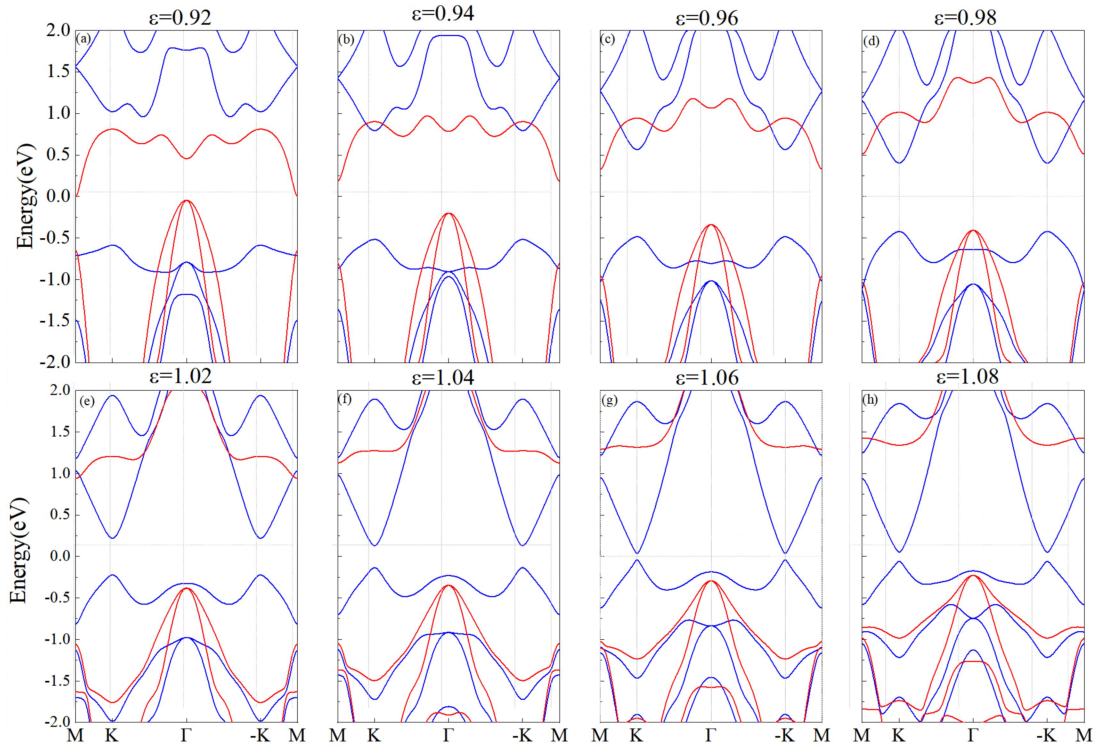

Fig. S9 The spin-polarized energy band diagram for the case where ε=0.92-1.08, with the Fermi level set to 0. Blue represents the spin-up energy bands, while red represents the spin-down energy bands.

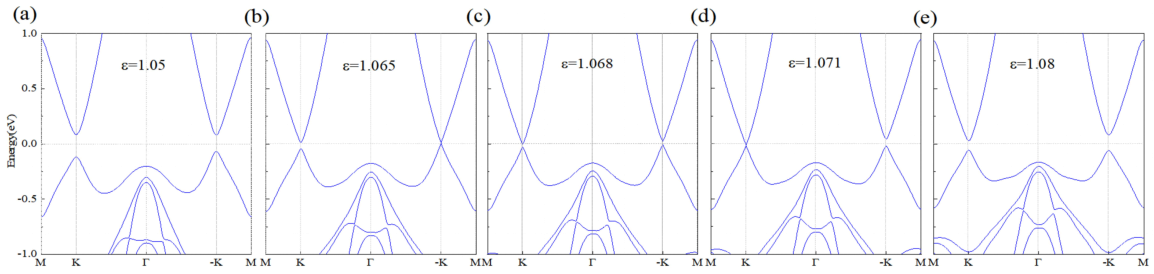

Fig.S10 The GGA+U+SOC energy bands of SVNH monolayer under representative biaxial strains, with the Fermi level set to 0.

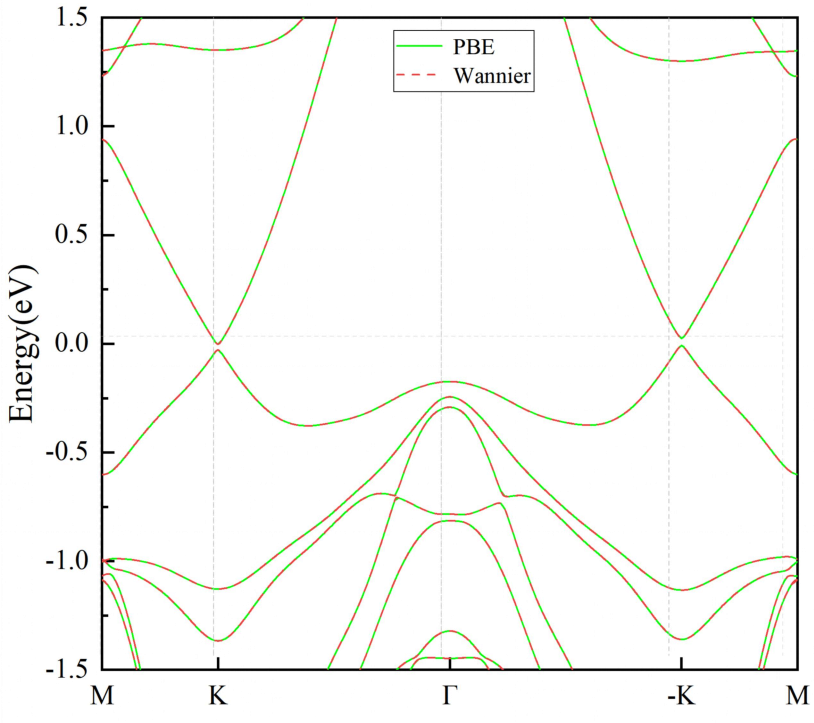

Fig. S11 The DFT and Wannier fitting energy bands of SVNH monolayer under 1.068 tensile strain, with the Fermi level set to 0.