Valley topological phase transitions under the combined effects of electronic correlation and strain in the H-TiSeBr monolayer

Xiangjie Chen^a, Yonghu Xu^a, Mengran Qin^a, Pei Zhang^b, Zhen Gao^{*a}, Yao He^{*a} and Kai Xiong^c

a Department of Physics, Yunnan University, Kunming 650091, People's Republic of China

b Hunan Provincial Key Laboratory of Intelligent Sensors and Advanced Sensor Materials, School of Physics and Electronics, Hunan University of Science and Technology.Xiangtan 411201, Hunan, P. R. China

c Materials Genome Institute, School of Materials and Energy, Yunnan University, Kunming 650091, People's Republic of China

* Authors to whom correspondence should be addressed: yhe@ynu.edu.cn, gao1323341943@163.com



FIG. S1 (a) The FM and (b) AFM configurations of the monolayer TiSeBr, (c) the energy difference between FM and AFM under different U_{eff}, and compared with HSE06.



FIG. S2 The curie-temperature from Monte Carlo simulations.



FIG. S3 The spin-polarized band structure calculated using the hybrid functional HSE06 is shown, where the red and green curves represent spin-up and spin-down states, respectively, with the Fermi level set to zero.



FIG. S4 (a) Phonon spectrum diagrams under a strain of $\varepsilon = -5\%$. (b) Phonon spectrum diagrams under a strain of $\varepsilon = 5\%$. (c) E_{MAE} under different strains. The E_{FM} and E_{AFM} under different bixial strain. Blue represents E_{AFM} , and red represents E_{FM} .



FIG. S5 Spin-resolved energy band diagrams considering SOC under strains of (a) $\varepsilon = -5\%$, (b) $\varepsilon = -3\%$, (c) $\varepsilon = -1.32\%$, (d) $\varepsilon = -1.24\%$, (e) $\varepsilon = -1.165\%$, (f) $\varepsilon = 1\%$, (g) $\varepsilon = 3\%$, and (h) $\varepsilon = 5\%$. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to



FIG. S6 Phonon spectrum diagrams under different Ueff.



FIG. S7 Spin-resolved energy band diagrams considering SOC under strains of (a) $U_{eff} = 2.2eV$, (b) $U_{eff} = 2.3eV$, (c) $U_{eff} = 2.4eV$, (d) $U_{eff} = 2.5eV$, (e) $U_{eff} = 2.6eV$. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to 0.



FIG. S8 Spin-resolved energy band diagrams considering SOC under strains of (a) U_{eff} = 2.7eV, (b) U_{eff} = 2.8eV, (c) U_{eff} = 2.9eV, (d) U_{eff} = 3.0eV, (e) U_{eff} = 3.1eV. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to 0.



FIG. S9 Spin-resolved energy band diagrams considering SOC under strains of (a) U_{eff} = 3.2eV, (b)

 U_{eff} = 3.3eV, (c) U_{eff} = 3.4eV, (d) U_{eff} = 3.5eV, (e) U_{eff} = 3.6eV. The spin-up and spin-down states

are represented by red and green lines, respectively. The Fermi level set to 0.



FIG. S10 Strain-tuned HVM and edge state energy bands under (a)-(c) $U_{eff} = 2.2 \text{ eV}$, (d)-(f) $U_{eff} = 2.3 \text{ eV}$, and (g)-(i) $U_{eff} = 2.4 \text{ eV}$. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to 0.



FIG. S11 Strain-tuned HVM and edge state energy bands under (a)-(c) $U_{eff} = 2.2 \text{ eV}$, (d)-(f) $U_{eff} = 2.3 \text{ eV}$, and (g)-(i) $U_{eff} = 2.4 \text{ eV}$. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to 0.



FIG. S12 Strain-tuned HVM and edge state energy bands under (a)-(c) U_{eff} = 2.2 eV, (d)-(f) U_{eff} = 2.3 eV, and (g)-(i) U_{eff} = 2.4 eV. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to 0.



FIG. S13 Strain-tuned HVM and edge state energy bands under (a)-(c) $U_{eff} = 3.1 \text{ eV}$, (d)-(f) $U_{eff} = 3.2 \text{ eV}$, and (g)-(i) $U_{eff} = 3.3 \text{ eV}$. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to 0.



FIG. S14 Strain-tuned HVM and edge state energy bands under (a)-(c) $U_{eff} = 3.4 \text{ eV}$, (d)-(f) $U_{eff} = 3.5 \text{ eV}$, and (g)-(i) $U_{eff} = 3.6 \text{ eV}$. The spin-up and spin-down states are represented by red and green lines, respectively. The Fermi level set to 0.