

Supplementary Information

High spin polarization, large perpendicular magnetic anisotropy and room-temperature ferromagnetism by biaxial strain and carrier doping in Janus MnSeTe and MnSTe

Long Zhang,^a Yan Zhao,^a Yuqi Liu,^a and Guoying Gao^{*a,b}

^aSchool of Physics, Huazhong University of Science and Technology, Wuhan 430074, China

^bWuhan National High Magnetic Field Center, Huazhong University of Science and Technology,

Wuhan 430074, China

*E-mail: guoying_gao@mail.hust.edu.cn

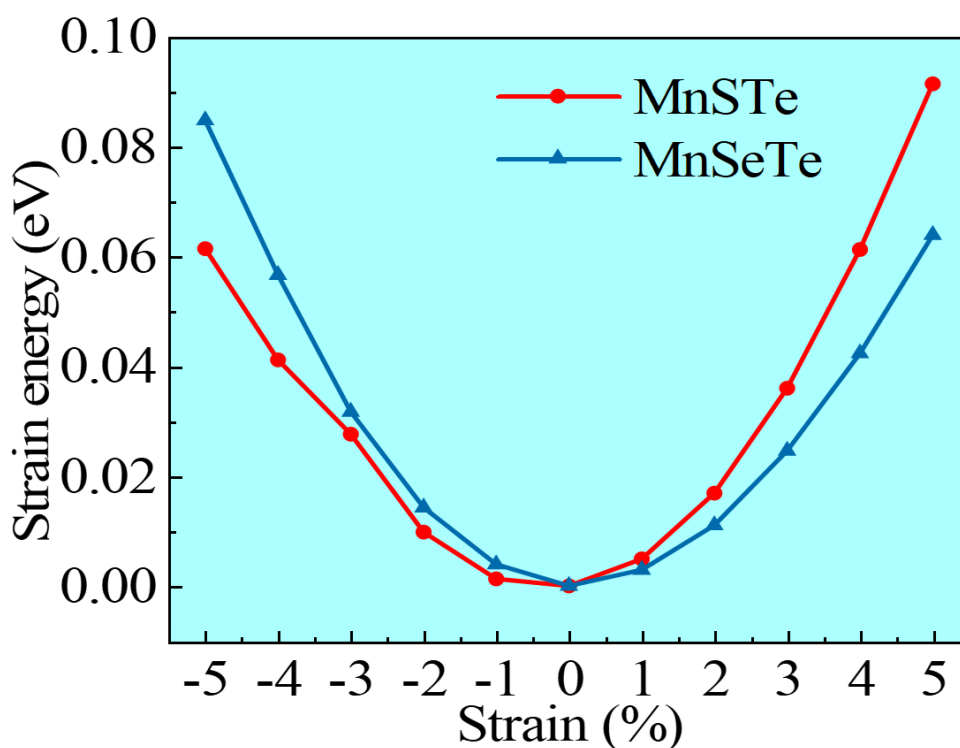


Fig. S1. The strain energies of monolayer MnSTe and MnSeTe under biaxial strain.

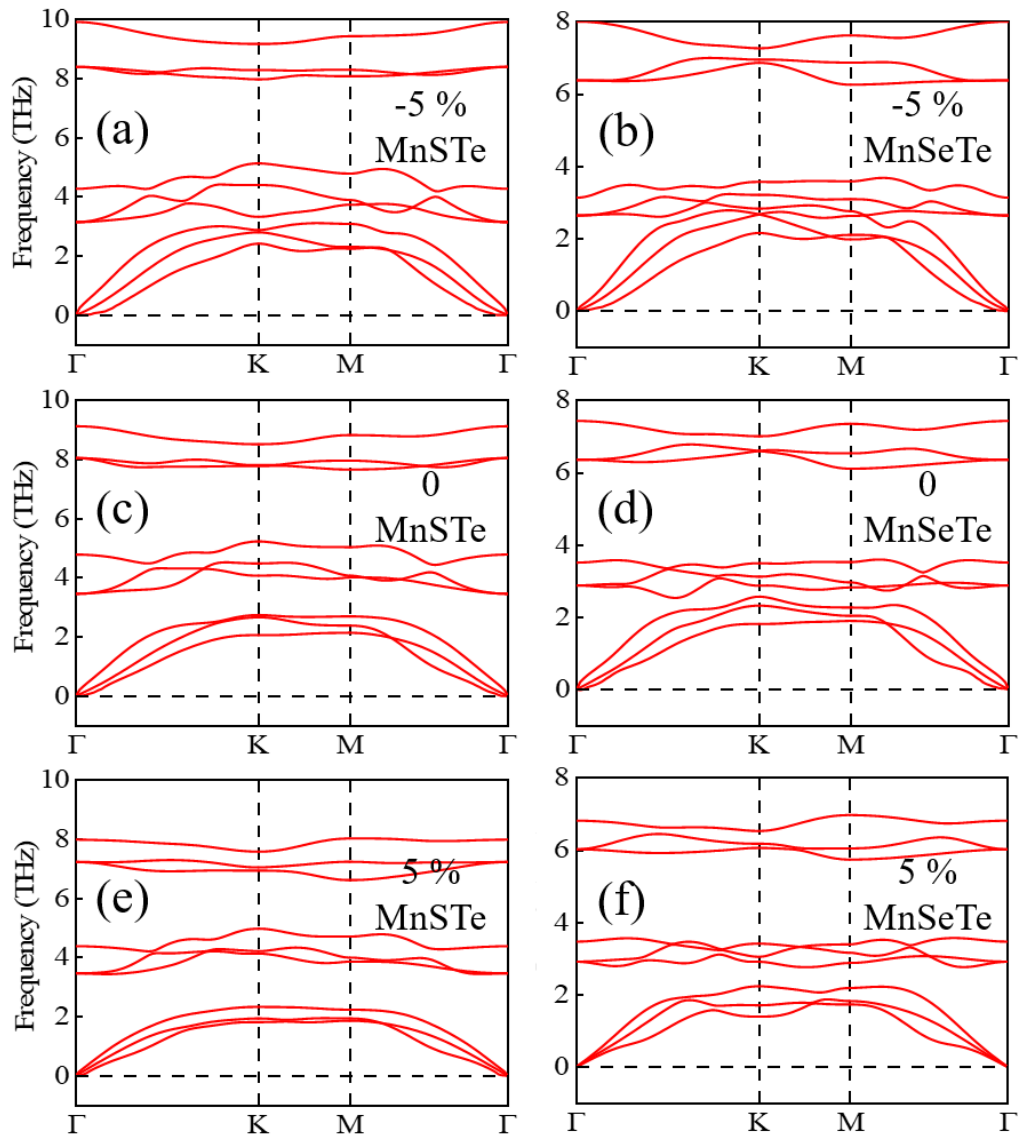


Fig. S2. Phonon dispersion of monolayer MnSTe and MnSeTe under -5 %, 0 and 5 % strain.

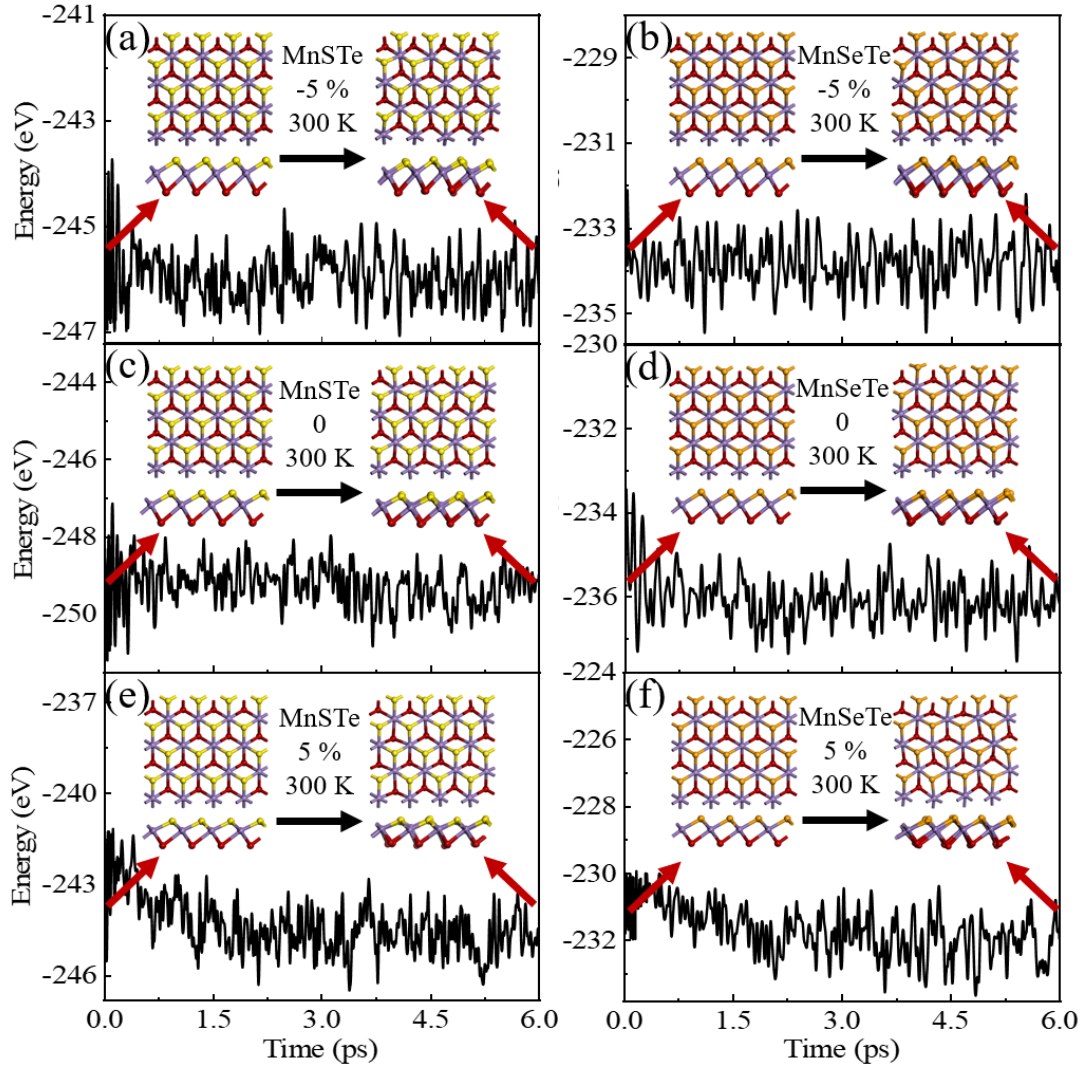


Fig. S3. The fluctuation of total energies and snapshots of geometric structures of monolayer MnSTe and MnSeTe under -5 %, 0 and 5 % strain.

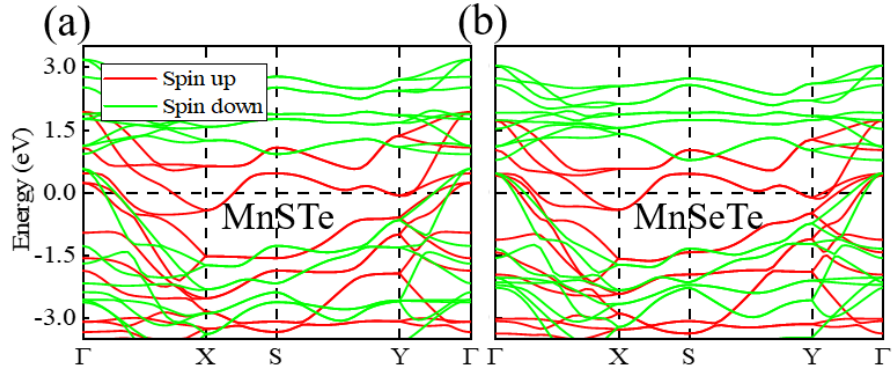


Fig. S4. The spin-dependent electronic band structures of monolayer MnSTe (a) and MnSeTe (b).

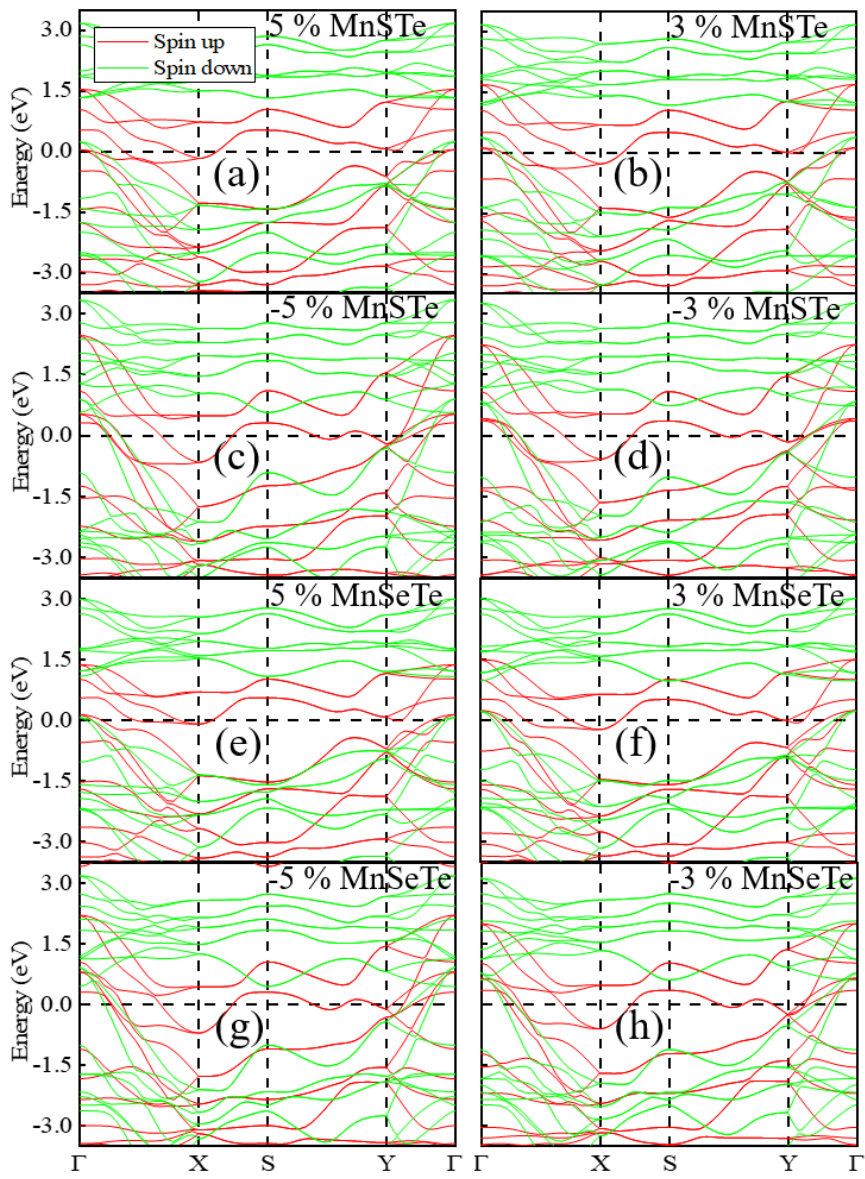


Fig. S5. The spin-dependent electronic band structures of monolayer MnSTe (a, b, c, d) and MnSeTe (e, f, g, h) with ferromagnetic state under various strains.

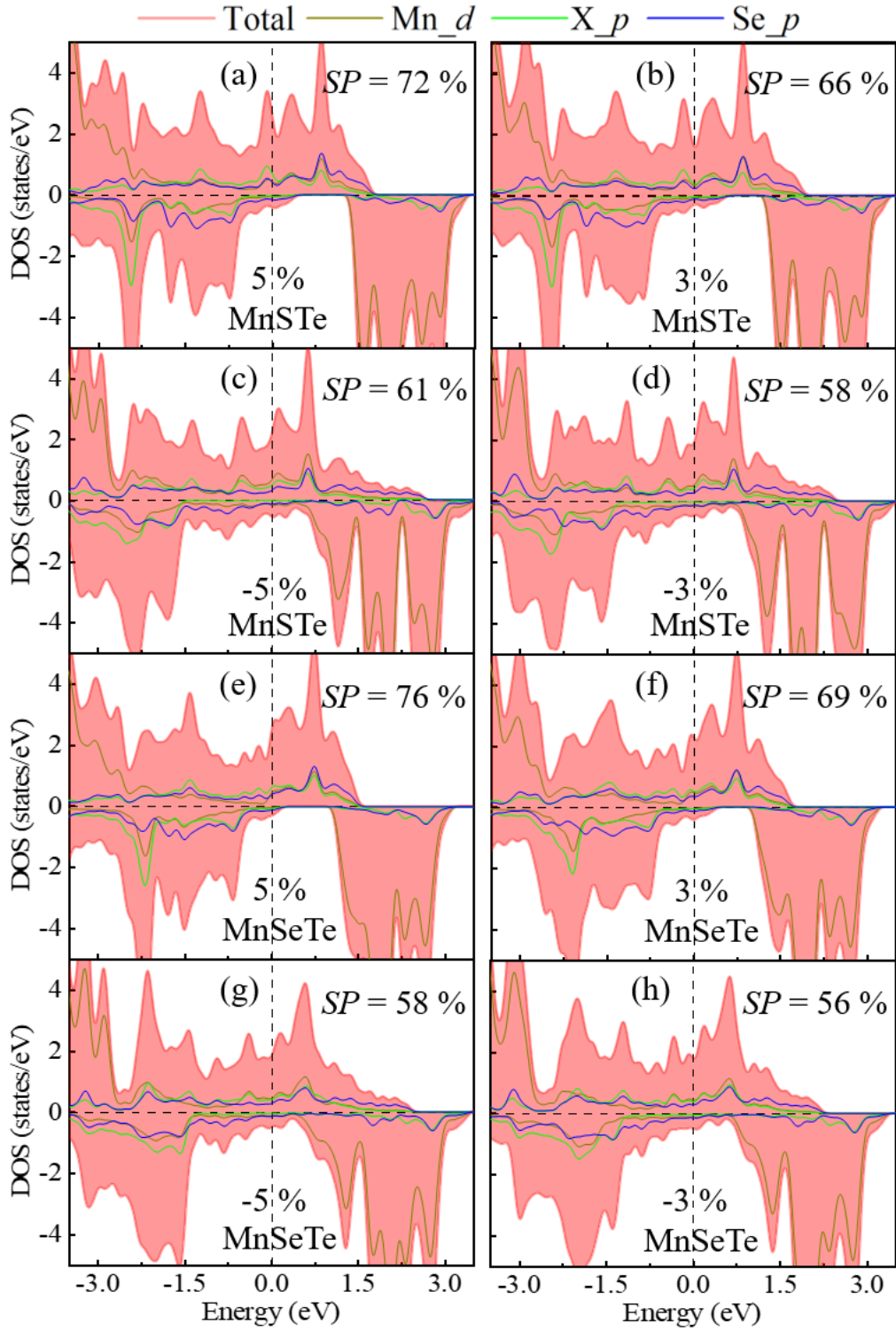


Fig. S6. The spin-dependent total and main projected DOSs of monolayer MnSTe (a, b, c, d) and MnSeTe (e, f, g, h) with ferromagnetic state under various strains.

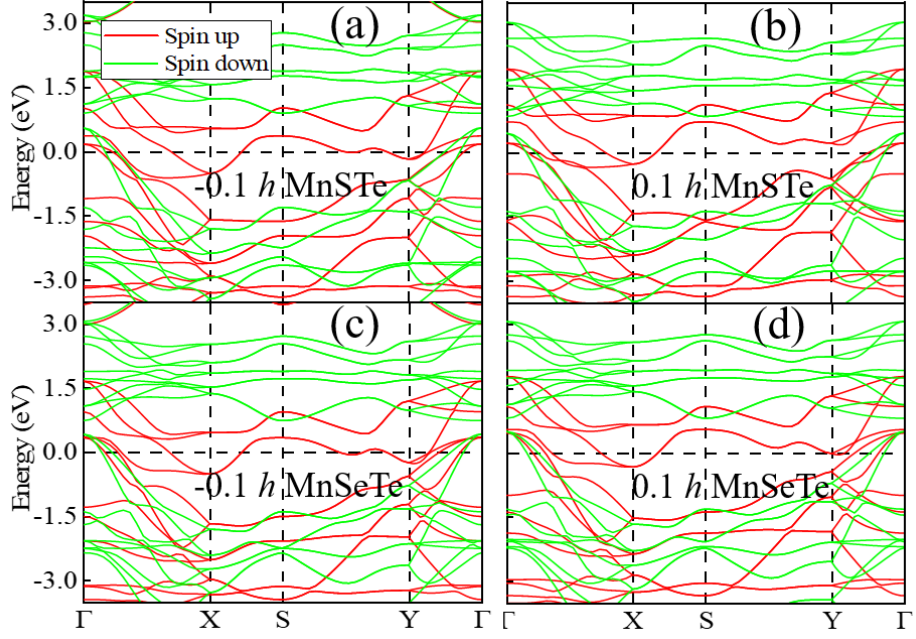


Fig. S7. The spin-dependent electronic band structures of monolayer MnSTe (a, b) and MnSeTe (c, d) with carrier doping.

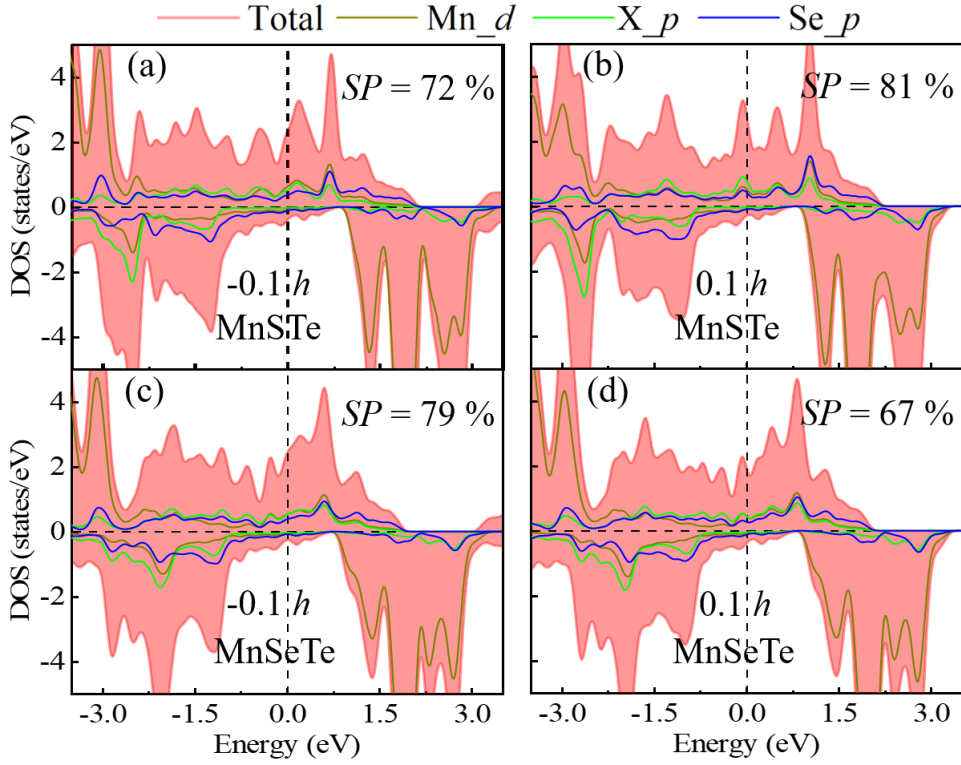


Fig. S8. The spin-dependent total and main projected DOSs of monolayer MnSTe (a) and MnSeTe (b) with carrier doping.

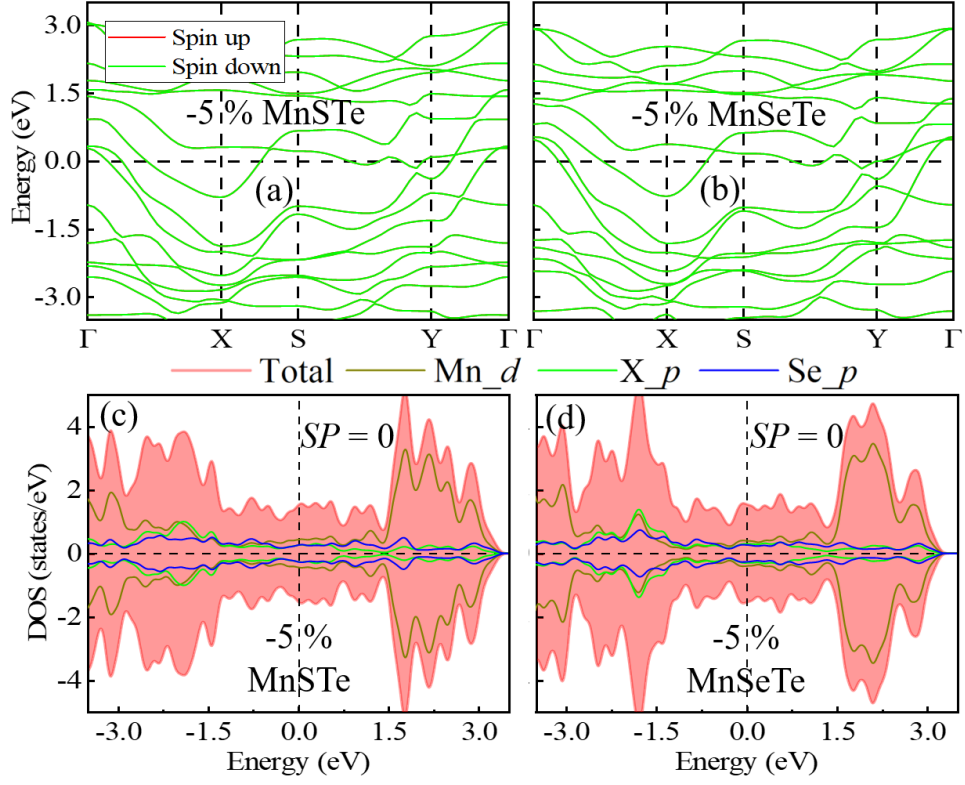


Fig. S9. The spin-dependent electronic band structures (a, b), total and main projected DOSs (c, d) of monolayer MnSTe and MnSeTe with antiferromagnetic state under the -5 % strain.

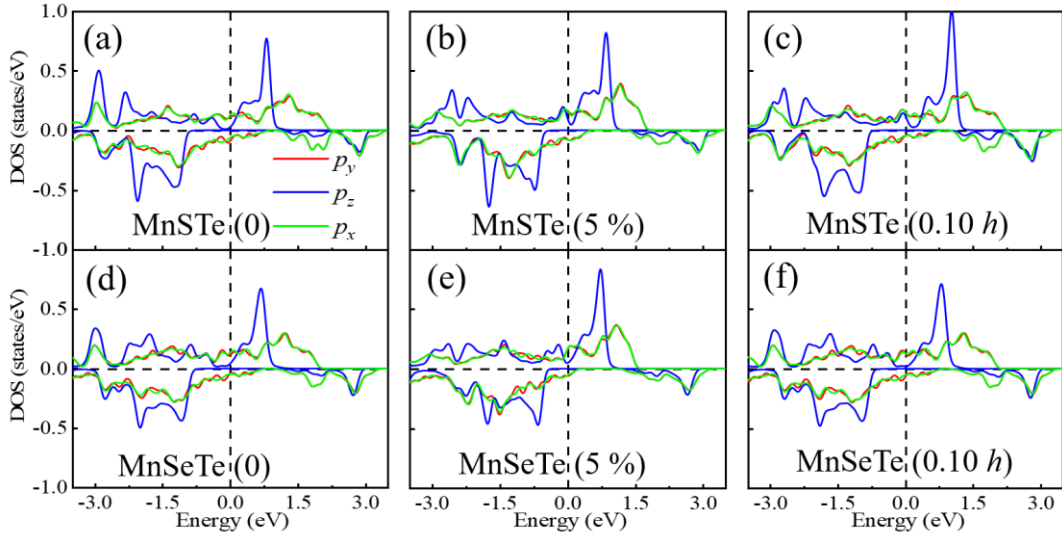


Fig. S10. Projected DOSs of Te- p orbitals of monolayer MnSTe (a,b,c) and MnSeTe (d,e,f) with 0, 5 % strain and 0.10 h doping.

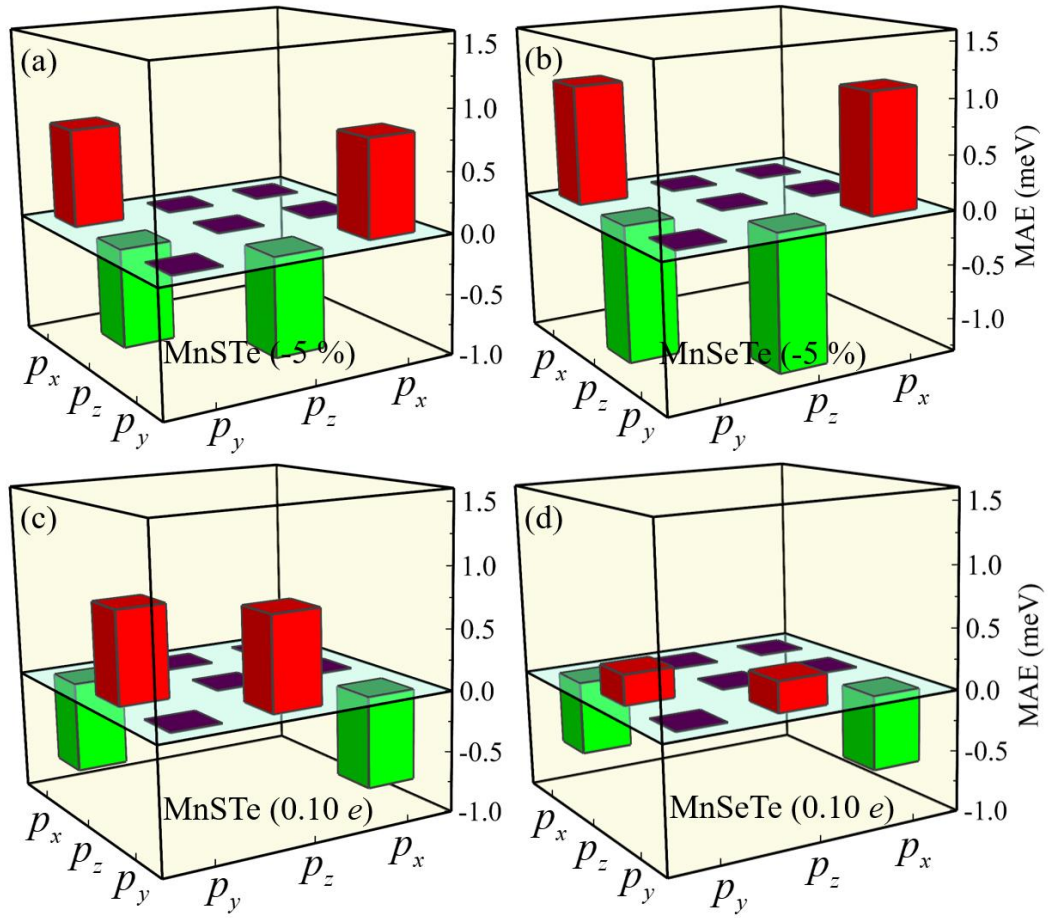


Fig. S11. MAE contributions from Te- p orbitals hybridization of monolayer MnSTe and MnSeTe with -5 % strain (a, b) and 0.10 e doping (c, d).

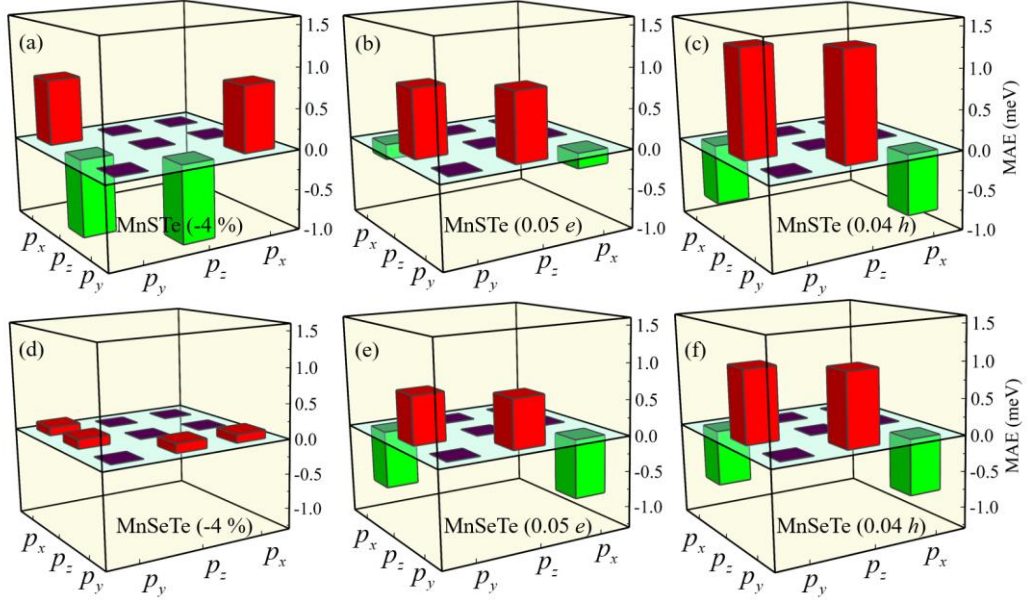


Fig. S12. MAE contributions from Te- p orbitals hybridization of monolayer MnSTe with -4 % strain (a), 0.05 e and 0.04 h doping (b, c), and monolayer MnSeTe with -4 % strain (d), 0.05 e and 0.04 h doping (e, f).

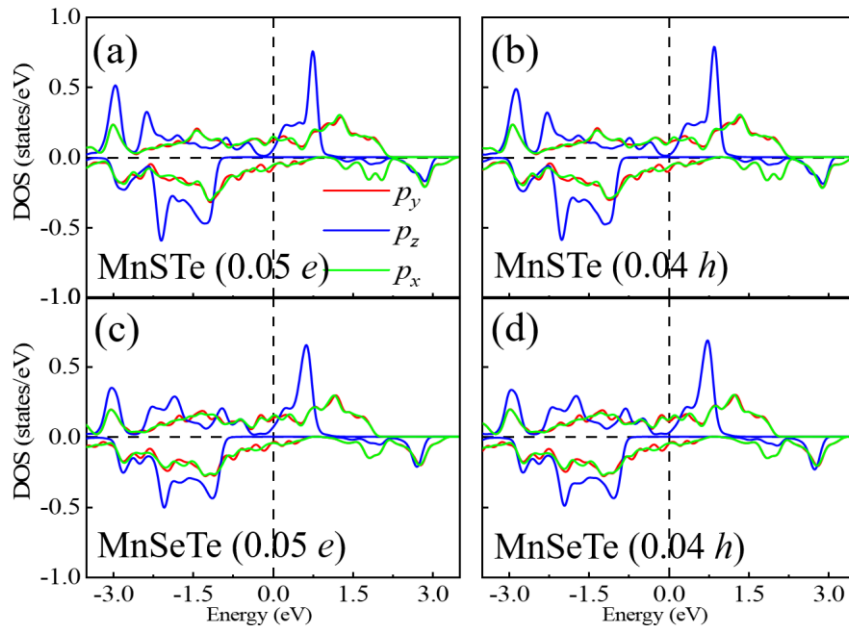


Fig. S13. Projected DOSs of Te- p orbitals of monolayer MnSTe (a,b) and MnSeTe (c,d) with 0.05 e and 0.04 h doping.

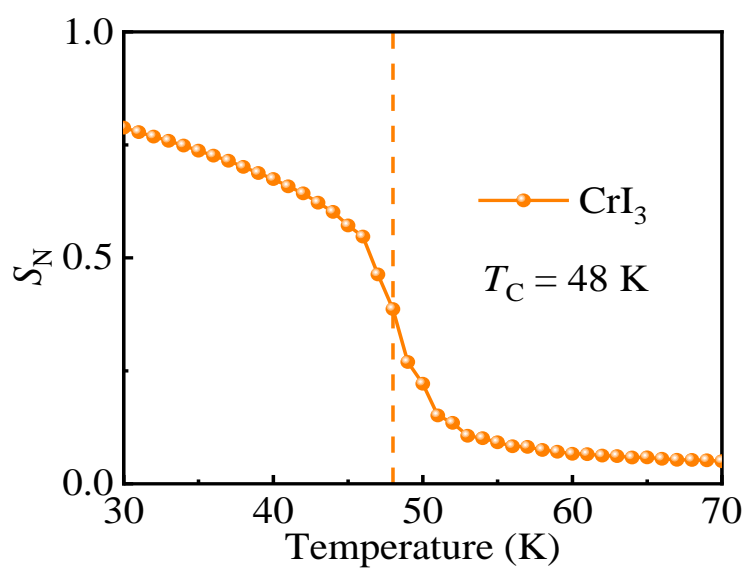


Fig. S14. The normalized spin operator (S_N) varying with the increasing of temperature for monolayer CrI₃.