Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Tunable Valley splitting and Anomalous Valley Hall Effect in Hole-doped WS_2 by Proximity Coupling with Ferromagnetic MnO_2 monolayer

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Table S1. The calculated lattice constant a, interfacial distance d (Å), binding energy E_b (eV), magnetic moments M (μ_B) of WS_2 and MnO_2 layers, and valley splitting ($\Delta_{KK'}$) of the heterostructures with different stacking configurations.

	Fcc-I	Fcc-II	Hcp-I	Hcp-II	Top-I	Top-II
a (Å)	3.08	3.09	3.06	3.06	3.09	3.07
d (Å)	2.74	2.71	2.77	2.76	3.19	3.24
E_b (eV)	-1.26	-1.35	-1.26	-1.28	-1.20	-1.21
M (WS_2)	0.058	0.065	0.055	0.055	0.023	0.025
M (MnO_2)	3.023	3.031	3.016	3.014	3.007	3.011
$\Delta_{KK'}$	17	43	35	39	21	15

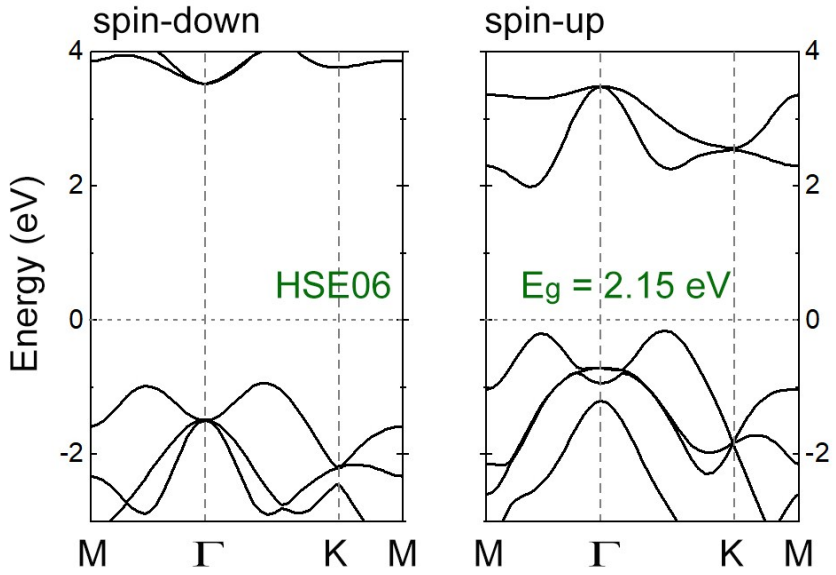

Fig. S1. Calculated band structure of pristine 2D MnO_2 by HSE06 method. The Fermi levels are set to zero.

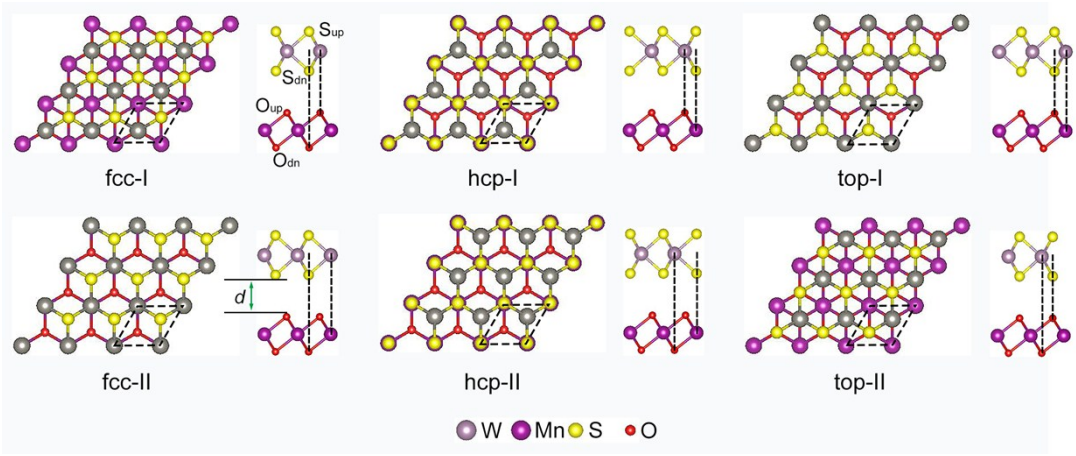

Fig. S2. Top and side views of WS_2/MnO_2 heterostructures with various stacking configurations.

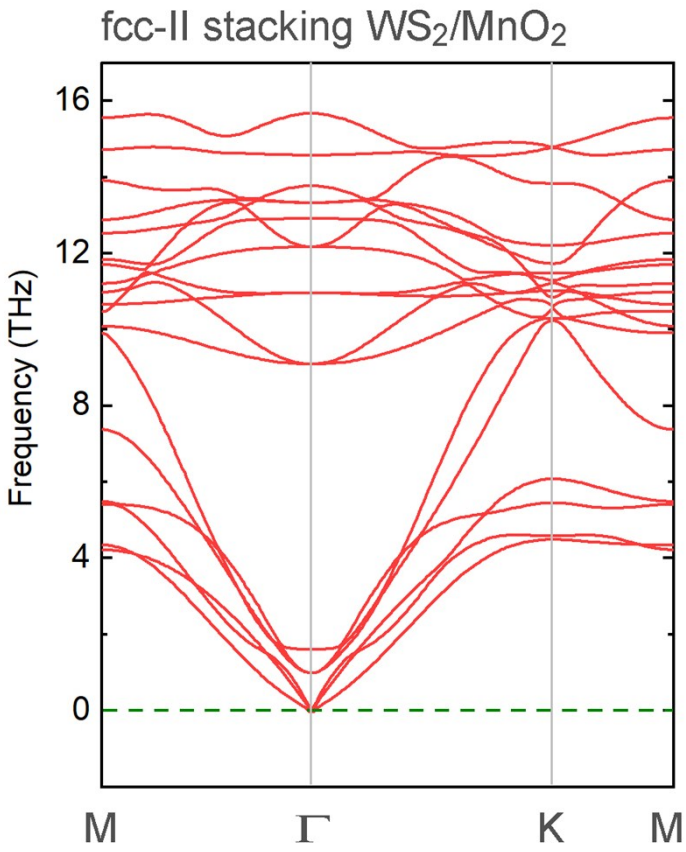

Fig. S3. Phonon bands of WS_2/MnO_2 heterostructure with fcc-II stacking model.

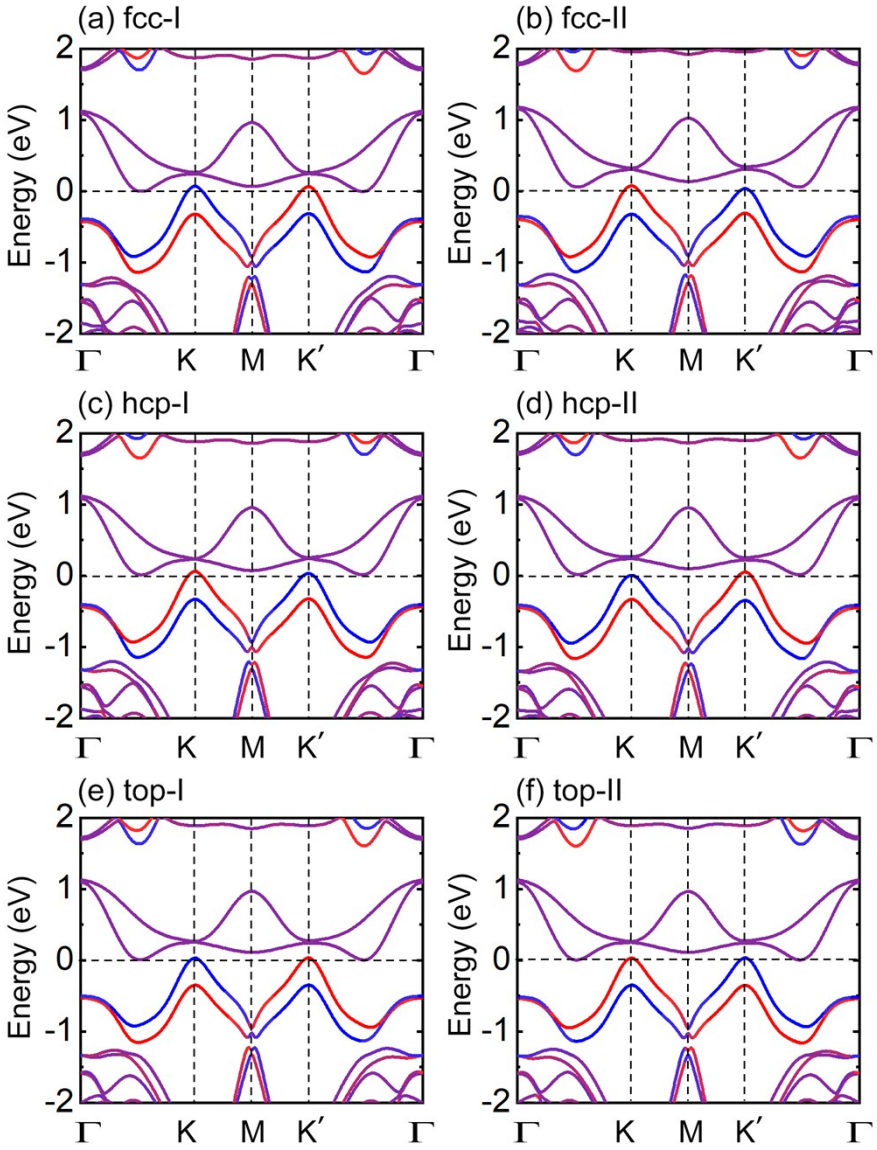

Fig. S4. Calculated band structures of the six configurations of WS_2/MnO_2 heterostructures. The spin projections for the WS_2 along *z* direction are represented by red and blue lines, which represent the spin-up and spin-down states, respectively. The Fermi level is set to zero.

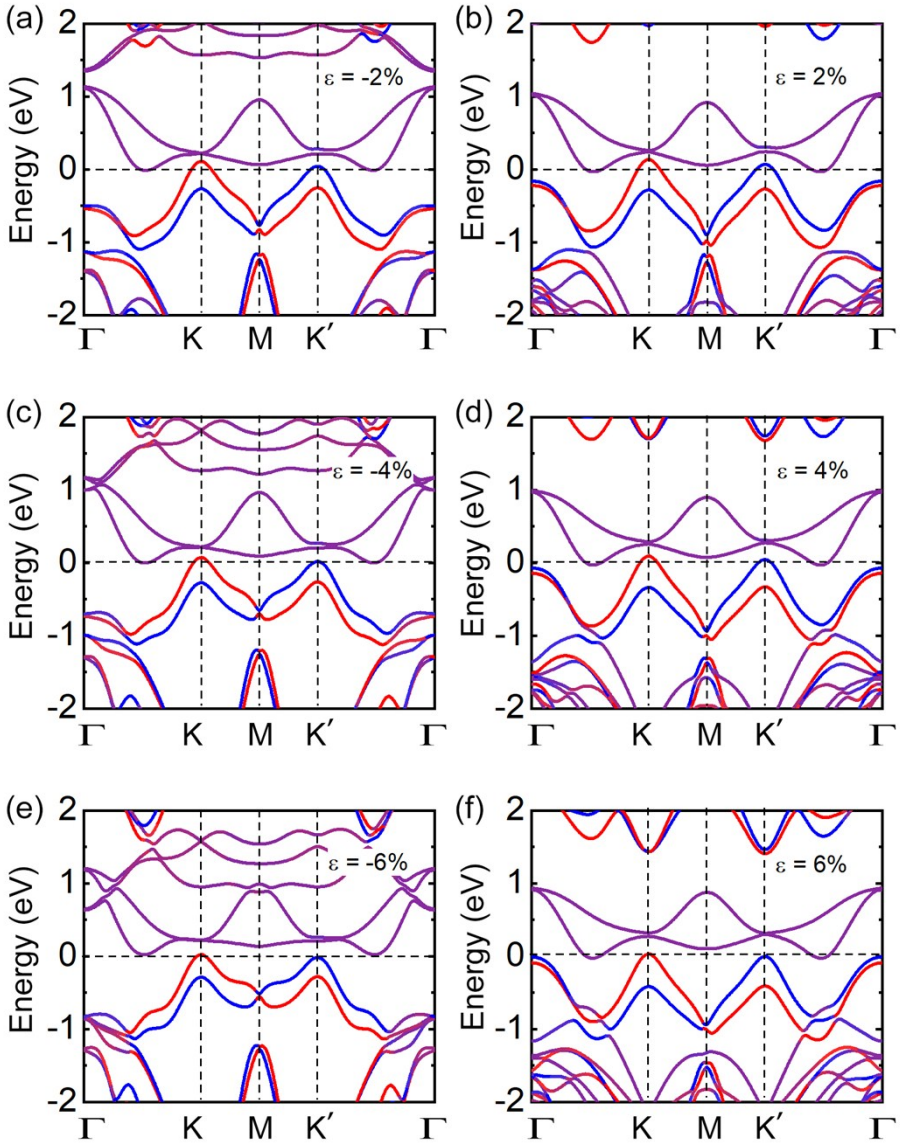

Fig. S5. Calculated band structures of fcc-II stacking WS_2/MnO_2 with various in-plane biaxial strain.