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

Supplementary Information

Superior Spin-Polarized Electronic Structure in MoS_2/MnO_2 Heterostructures with An Efficient Hole Injection

Baozeng Zhou*, Zheng Li, Jiaming Wang, Kangqiang Wang

Tianjin Key Laboratory of Film Electronic & Communicate Devices, School of Electrical and Electronic Engineering, Tianjin University of Technology, Tianjin 300384, China

*Author to whom all correspondence should be addressed.

E-mail: baozeng@tju.edu.cn

Table S1. Calculated lattice constant a, M-X bond length ($d_{M\text{-}X}$), layer thickness ($d_{X\text{-}X}$), interlayer distance D, energy difference (ΔE) between FM and AFM states, magnetic moments (Mag), and work function (Φ) of the pristine monolayers and the most stable most stable configurations in each group.

	a (Å)	$d_{M\text{-}X}$ (Å)	$d_{X\text{-}X}$ (Å)	D (Å)	ΔE (meV)	Mag (μ_B)	Φ (eV)
h-MnO_2	2.90	1.85	2.31	–	38	0.66	6.31
t-MnO_2	2.98	1.88	2.50	–	53	3.00	6.98
MoS_2	3.13	2.37	3.12	–	–	0.00	5.85
MoS_2/$h$$MnO_2$	3.05	–	–	2.79	45	1.20	5.96
MoS_2/$t$$MnO_2$	3.06	–	–	2.76	49	3.00	6.32

Table S2. In-plane lattice constant a, equilibrium interlayer distance D, and binding energies (E_b) of all stacking models.

MoS_2/h-MnO_2	AA	AB	C27	C28	T1	T2
a (Å)	3.05	3.05	3.03	3.05	3.06	3.05
D (Å)	3.21	2.79	2.86	3.18	2.83	2.80
E_b (meV)	-133.7	-296.5	-239.2	-138.3	-221.7	-243.6
MoS_2/t-MnO_2	fcc-I	fcc-II	hcp-I	hcp-II	top-I	top-II
a (Å)	3.06	3.06	3.05	3.06	3.06	3.06
D (Å)	2.80	2.76	2.82	2.86	3.29	3.27
E_b (meV)	-312.3	-337.8	-309.2	-303.7	-180.7	-188.6

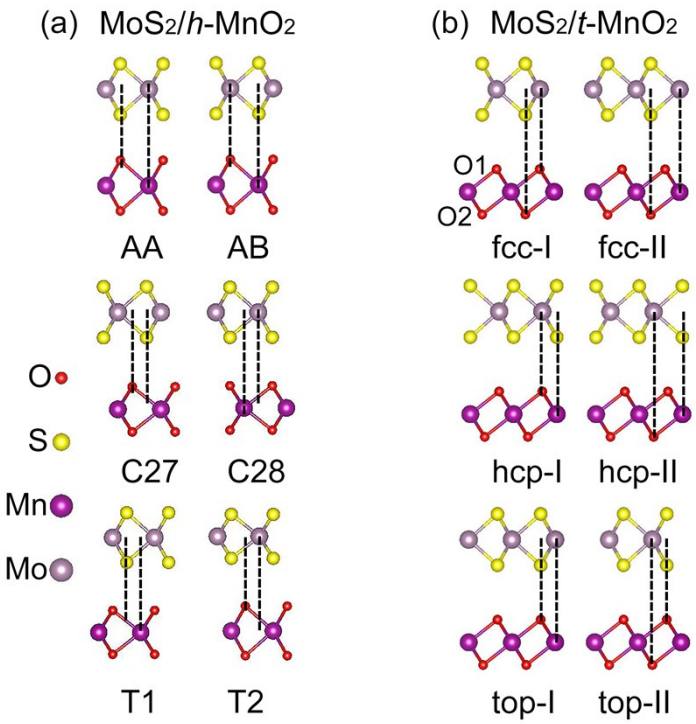

Fig. S1. Side views of the nonequivalent configurations of (a) MoS_2/*h*-MnO_2 and (b) MoS_2/*t*-MnO_2 heterostructures.

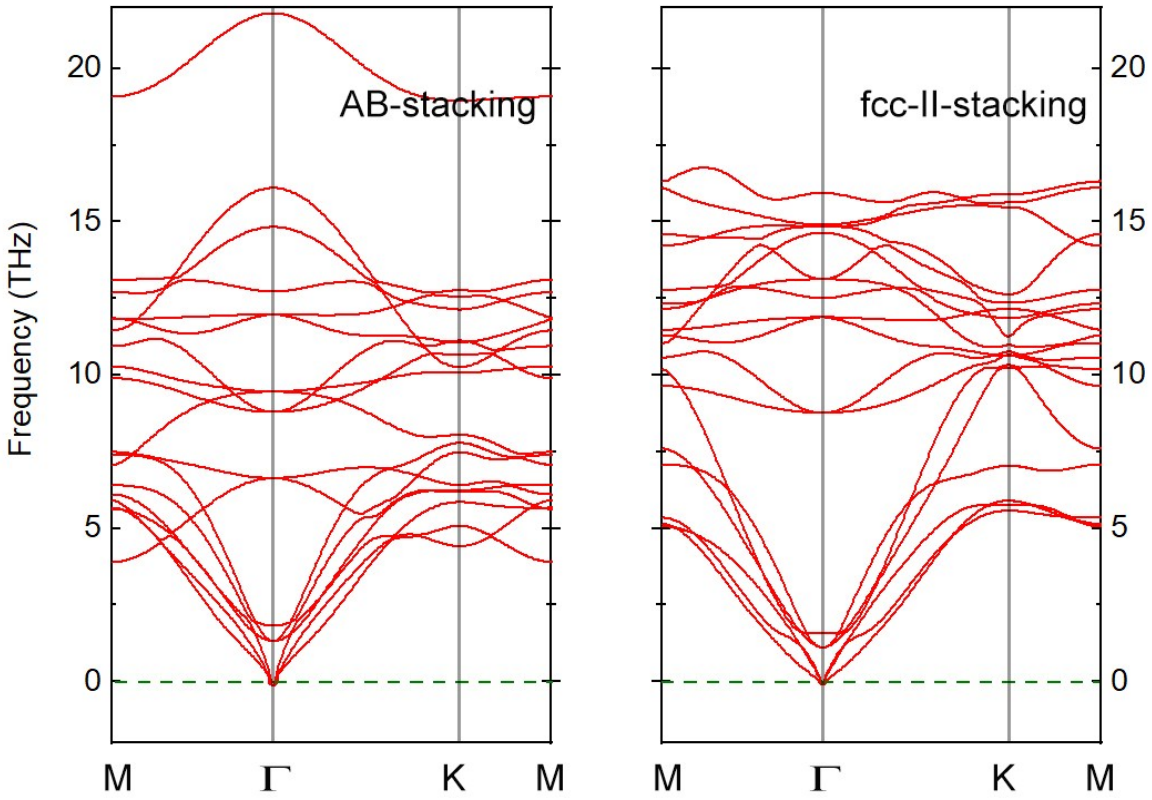

Fig. S2. Phonon bands of AB and fcc-II stacking models.

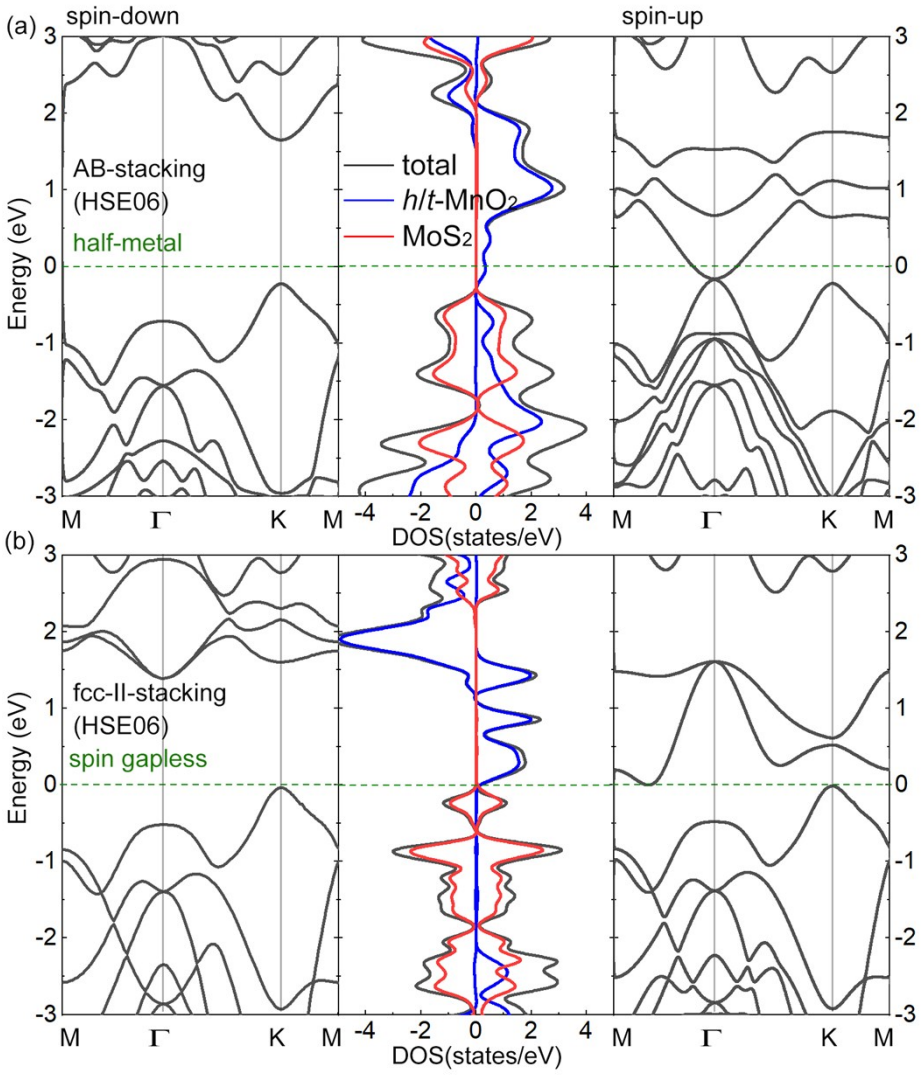

Fig. S3. The calculated band structures and DOS by HSE06 methods for (a) AB and (b) fcc-II stacking heterostructures, respectively. The Fermi levels are set to zero.

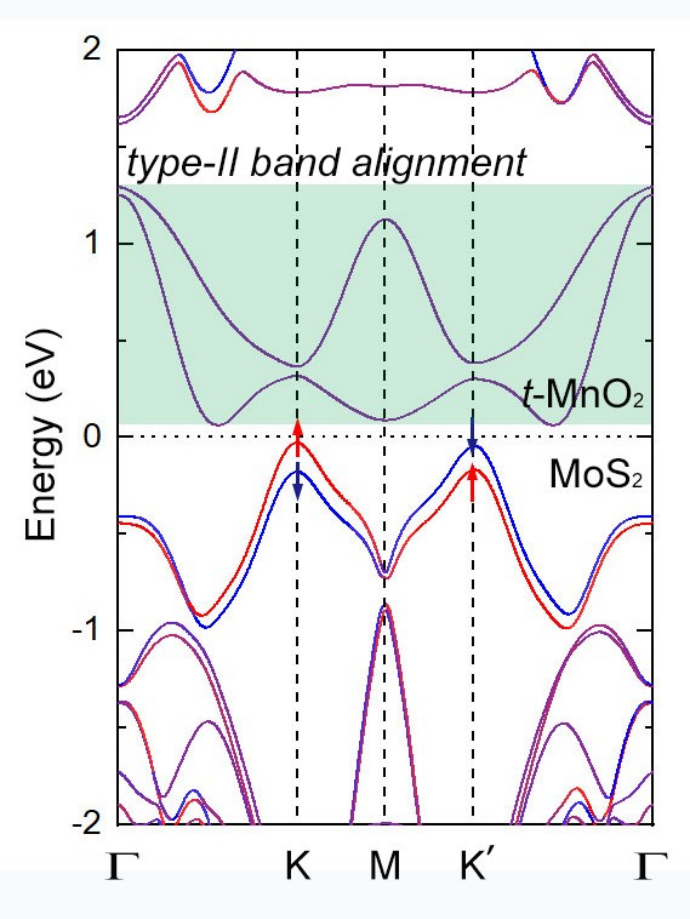

Fig. S4. Valley polarization in MoS_2/*t*-MnO_2 heterostructure. Spin-up and spin-down states are presented by red and blue, respectively.

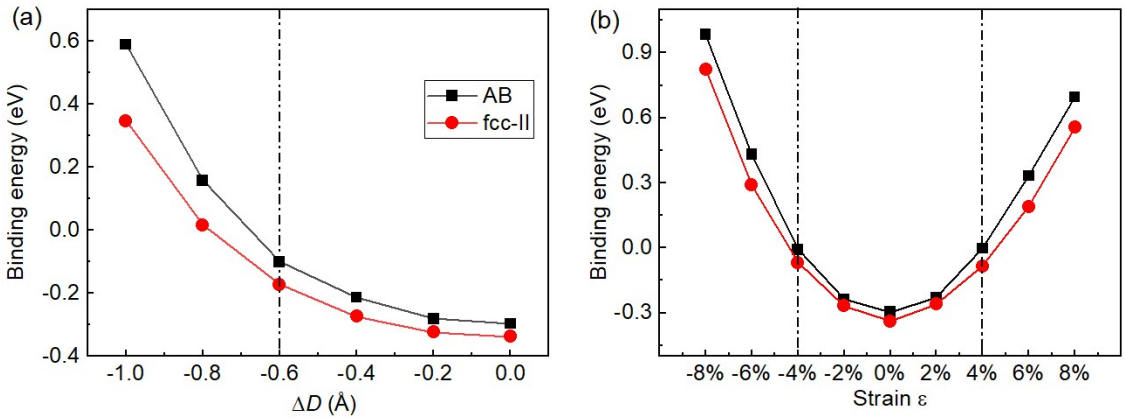

Fig. S5. Binding energies per unit cell as a function of (a) the interlayer distance and (b) in-plane strain in AB and fcc-II stacking heterostructures.

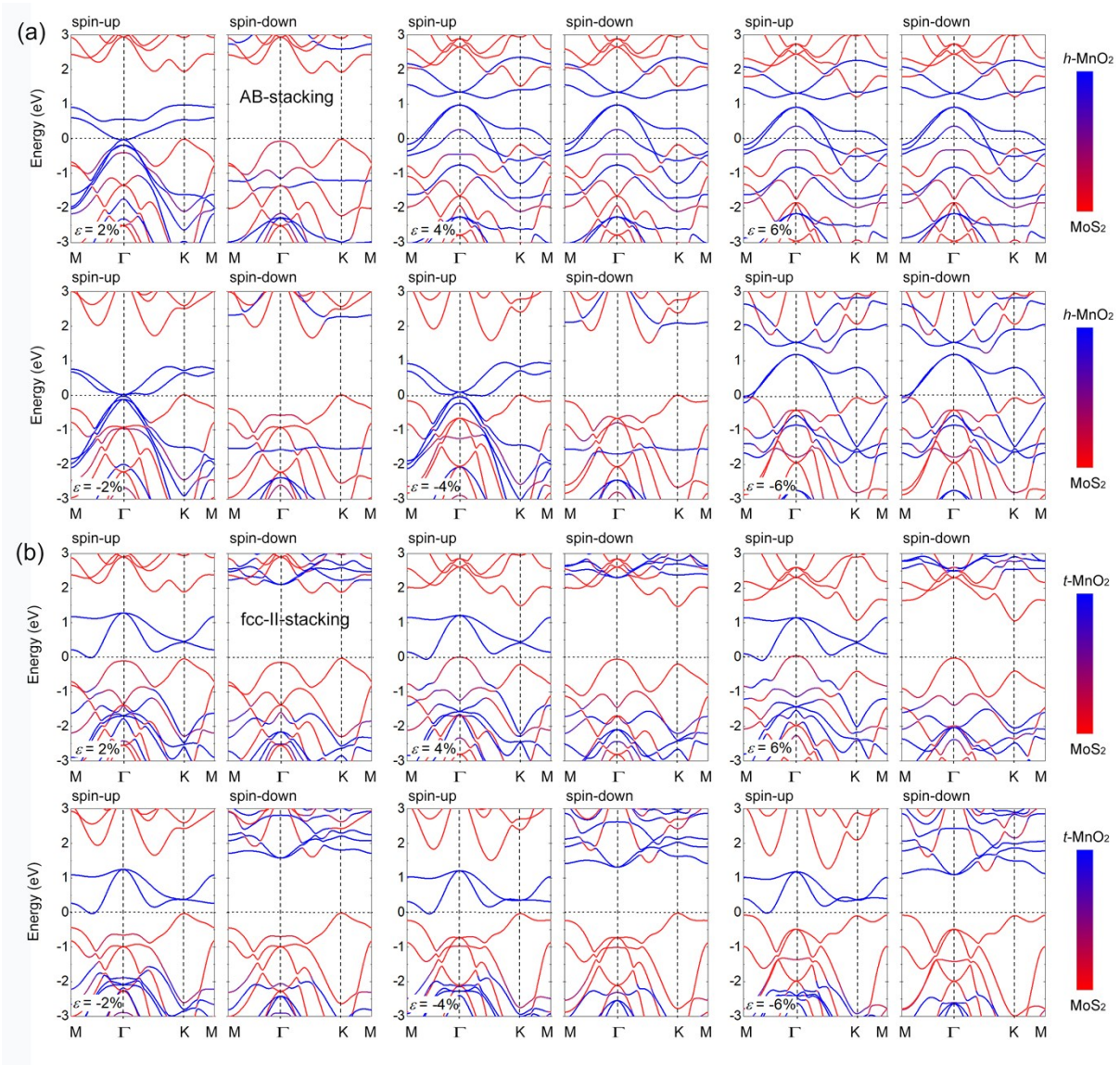

Fig. S6. Band structures of (a) AB-stacking and (b) fcc-II stacking models with varying in-plane biaxial strain. The Fermi level is set to zero.