Supporting Information

Mechanisms of manipulating valley splitting in $MoTe_2/MnS_2$ van der Waals heterostructure by electric field and strains

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Discussion of the results of $MoTe_2/MnS_2$ heterostructure with the relationship between interlayer spacing and magnetic moment.

We have investigated the magnetic moment of Mo dependence on layer spacing in four configurations. We calculated the energy band structure of the heterojunction at layer spacings of 2.5 A,2.75 A,3 A,3.25 A,3.5 A. The relationship between layer spacing and magnetic moment was obtained as shown in Fig. S1(a), and we observed that the smaller the layer spacing is, the larger the magnetic moment is in the same configuration. And there is a corresponding relationship between the value of valley splitting and magnetic moment, so we calculated the relationship between layer spacing and valley splitting using AB configuration as an example. As shown in Fig. S1(b), when the layer spacing is smaller, the magnetic moment is larger and the value of valley splitting is larger.

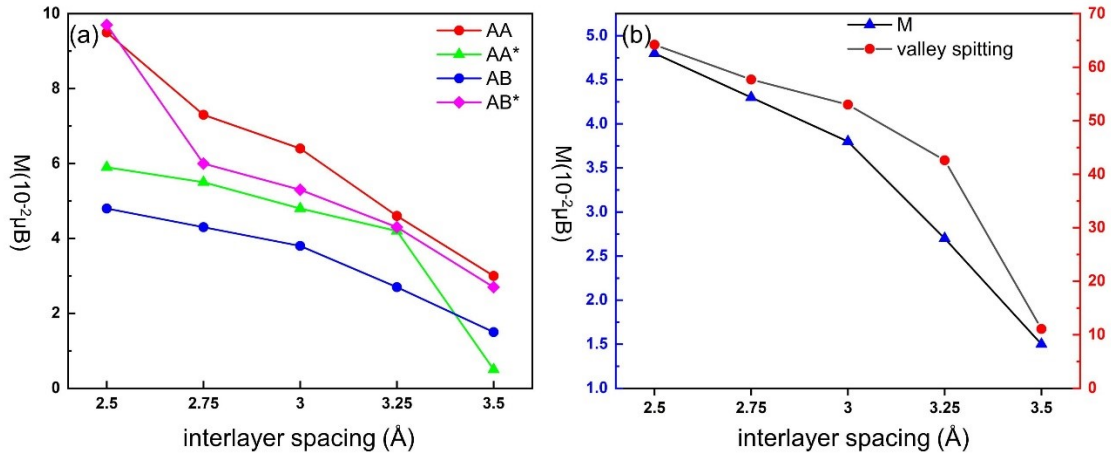

Fig. S1. (a) Relationship between interlayer spacing and magnetic moment for four configurations. (b) Relationship between layer spacing and valley splitting in AB configurations

Discussion of the results of $MoTe_2/MnS_2$ heterostructure with applied biaxial strain

Strain is a means by which the properties of two-dimensional materials can be effectively controlled, and a large number of previous reports have explored the effects of applied axial or in-plane and out-of-plane strains on the magnetic and electronic structure of TMDs materials, with applications in the fields of spintronics, optoelectronics, and so on.[1-3] When calculating heterostructure with different strains, we keep the heterostructure structure unchanged and only change the lattice constants for the correctness of the results. As shown in Fig. S2 are the projected energy band diagrams for strains of 1%, 2%, 3%, -1%, -2% and -3%, respectively. The red, pink, green, and blue parts represent the energy bands contributed by Mo, Te, Mn, and S atoms, respectively. When the strain goes from -3% to 3%, the band gap of the energy bands contributed by $MoTe_2$ decreases gradually, and the conduction bands at the K and K' valleys approach the Fermi energy level. From the energy band diagrams, the values of valley splitting can be read as 54.2meV, 52.9meV, 50.8meV, 56.5meV, 57.4meV, and 57.4meV at strains of 1%, 2%, 3%, -1%, -2%, and -3%. as shown in Fig. S3(a), which demonstrates the density of the projected states at three strains, 3%, 0%, and -3%, which corresponds to the energy band computed results correspond to the results. As shown in Fig. S3(b), the electrostatic potentials at 3%, 0%, and -3% strains are demonstrated, and the positive direction of the electrostatic potential-induced spontaneous internal electric field in the heterojunction is directed from the $MoTe_2$ layer to the MnS_2 layer.

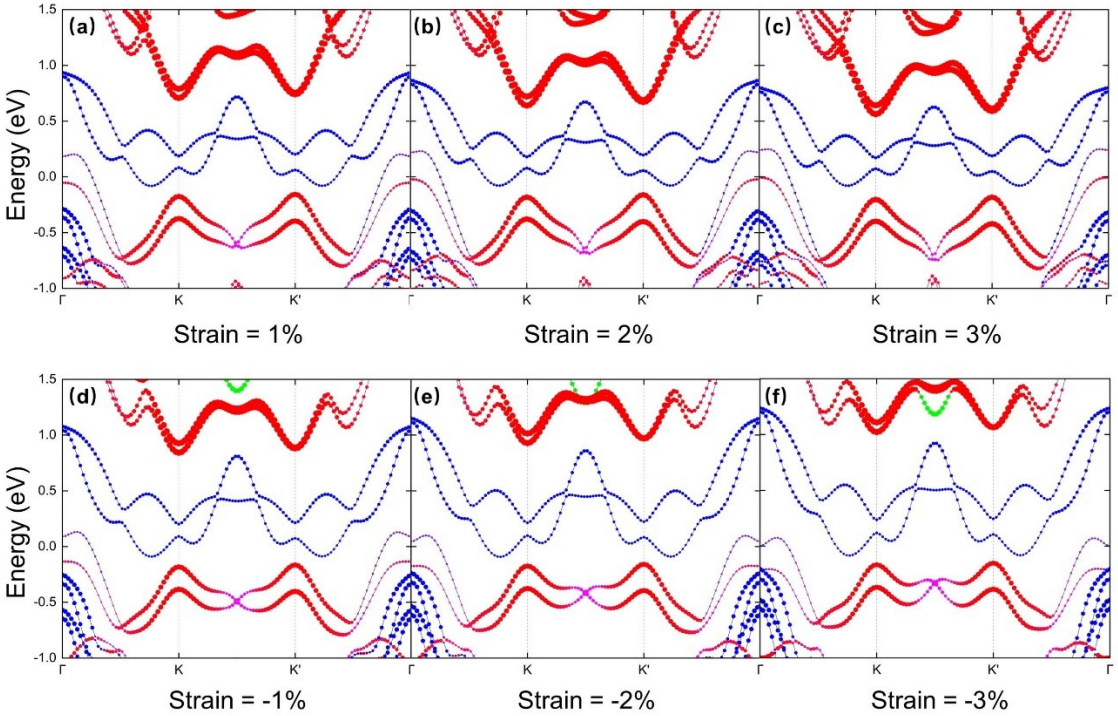

Fig. S2. (a)-(f) Band structure of the $MoTe_2/MnS_2$ heterostructure at 1%, 2%, 3%, -1% -2%, -3%.

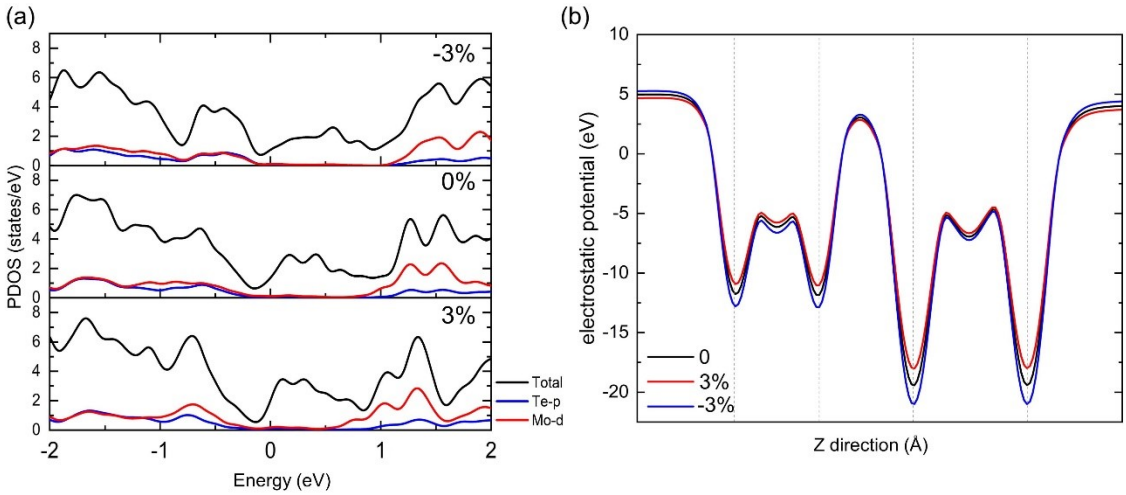

Fig. S3 (a) Projected density of states (PDOS) of the $MoTe_2/MnS_2$ heterostructure. (b) Electrostatic potential under different strains

Discussion of the results of $MoTe_2/MnS_2$ heterostructure with applied electric field

Applying an external electric field is an easily achievable method to control the electronic structure or valley properties[4]. As shown in Fig. S4, we show the projected energy band diagrams with different positive and negative electric fields applied. When the applied electric field is varied from -3V/Å to +3V/Å, we find that the energy band structure does not change much, but the value of the valley splitting decreases from 56.6meV to 49.2meV. The projected density of states for the $MoTe_2/MnS_2$ heterostructure with -3V/Å, 0V/Å, and +3V/Å electric fields applied to the heterostructure are demonstrated in Fig. S5(a). The electrostatic potentials under -3 V/Å, 0 V/Å, and +3 V/Å electric fields are shown in Fig. S5(b).

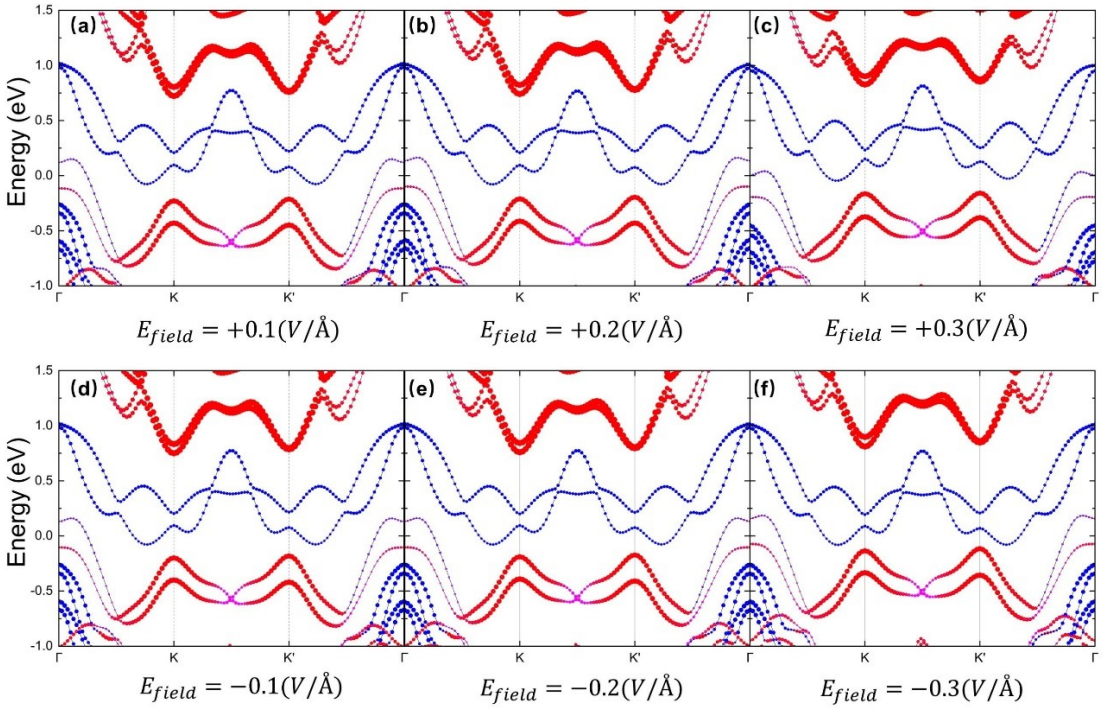

Fig. S4. (a)-(f) Band structure of the $MoTe_2/MnS_2$ heterostructure at +0.1V/Å, +0.2V/Å, +0.3V/Å, -0.1V/Å, -0.2V/Å, -0.3V/Å.

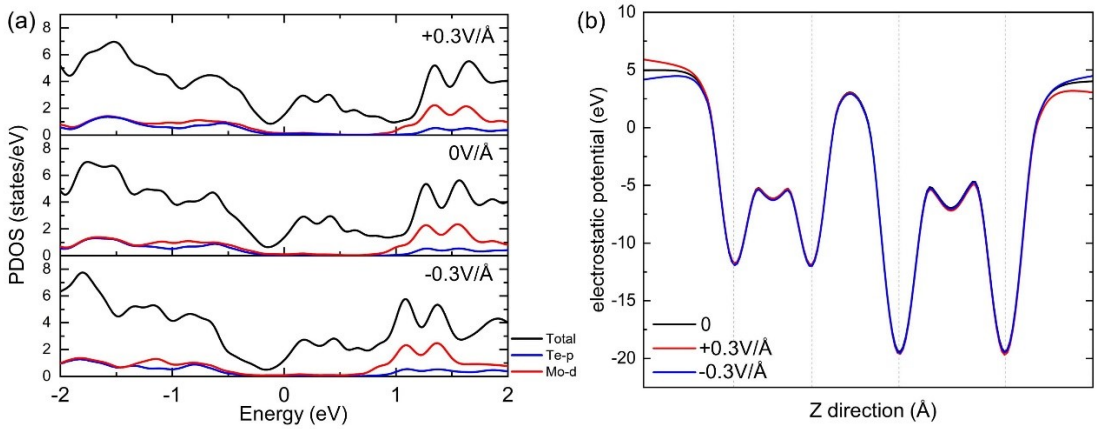

Fig. S5 (a) Projected density of states (PDOS) of the $MoTe_2/MnS_2$ heterostructure. (b) Electrostatic potential under different electric field.

Reference

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