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

Supporting Information for

Tunneling electroresistance effect in van der Waals ferroelectric tunnel junction based on graphene/In_2Se_3/MoS_2/graphene heterostructure

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1. **Comparison of the results calculated by two software**

To verify the consistency of the calculation results between the two software, we calculate the electronic band structures of monolayer In_2Se_3 [see Fig.S1(a) and (b)] and MoS_2 [see Fig.S1(c) and (d)] using the Vienna ab initio simulation package (VASP) and Nanodcal package. Their band structures are basically the same, but there are differences in the band gaps. Specifically, we observe that the band gaps calculated using the Nanodcal are always larger than those obtained from the VASP. while the results calculated using the Nanodcal are closer to the experimental values. The experimental band gap values for In_2Se_3 and MoS_2 are 1.39 eV[1] and 1.83 eV,[2] respectively. This is because VASP and the Nanodcal use different basis sets and pseudopotentials. The Nanodcal uses the double-ζ polarized (DZP) atomic-orbital basis and Troullier–Martins pseudopotentials.[3,4] VASP uses a plane wave basis set and projector-augmented-wave potentials.

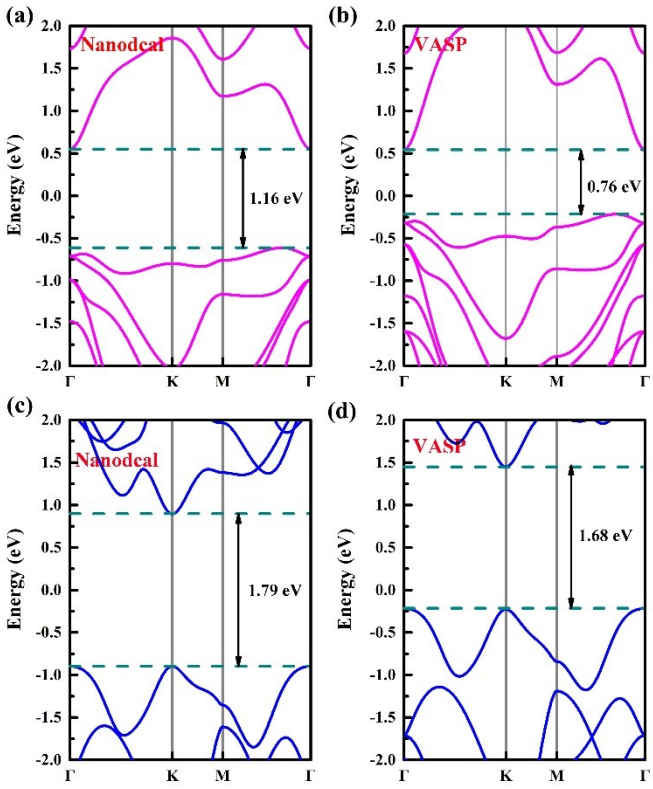

Fig. S1 The band structures of monolayer In_2Se_3 [(a) and (b)] and MoS_2 [(c) and (d)].

2. Other supporting results

We use the VASP to calculate the band structures of In_2Se_3/MoS_2 vdW heterostructures. In the $P_{\uparrow}$ state of the In_2Se_3/MoS_2 system, it is evident that the conduction band minimum (CBM) and valence band minimum (VBM) are mainly contributed by In_2Se_3, having an indirect band gap of 0.94 eV. As a result, the band structure displays a quasi type-I band alignment. When the polarization of In_2Se_3 is reversed, the band alignment is also changed from type-I to type-II. This also leads to a reduction in the band gap to 0.42 eV, where the In_2Se_3 layer contributes to the CBM and the MoS_2 layer contributes to the VBM.

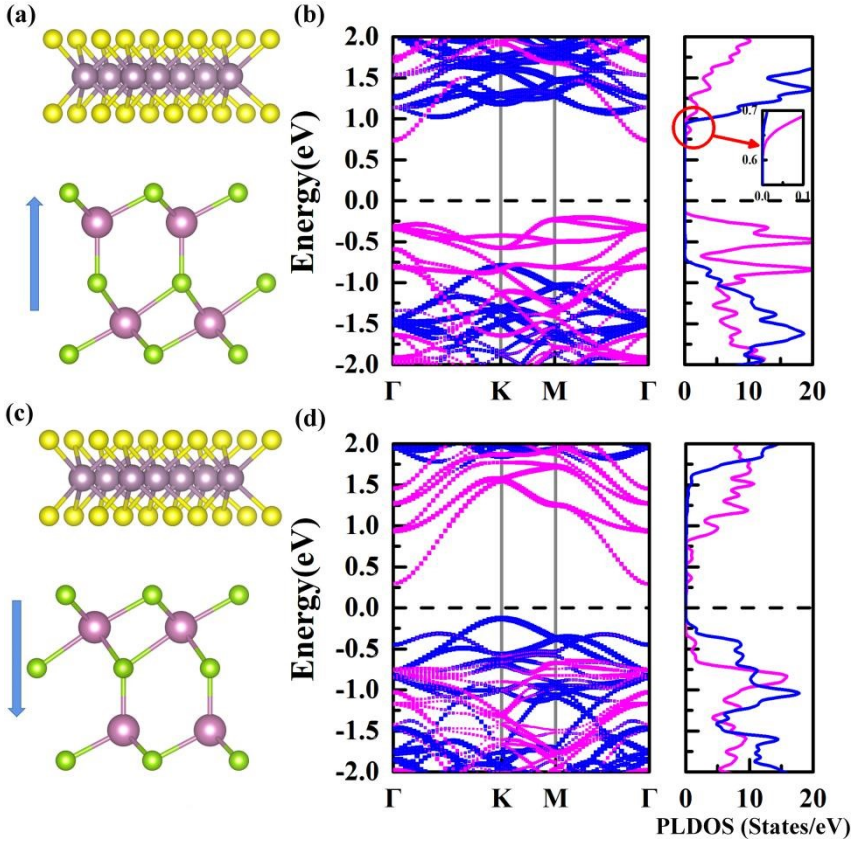

Fig. S2 Side view (a) and (c) of In_2Se_3/MoS_2 heterostructures, the blue arrows indicate the direction of out-of-plane electric polarization in In_2Se_3 layer. Projected band structures and the projected density of states for (b) In_2Se_3/MoS_2-↑ and (d) In_2Se_3/MoS_2-↓ calculated by using VASP method. The cyan lines represent contributions from the MoS_2 layer and magenta lines represent the In_2Se_3 layer.

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