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

Supporting Information

S1. The band structure difference between the results calculated by PBE and HSE06 functionals and its effect on the results of NEGF.

Compared with the band gaps of AA-P↑ and AA-P↓ calculated by HSE06 in Fig. 3(c-d), those calculated by PBE show much smaller band gaps as shown in Fig. S1. Specifically, the band gap of AA-P↑ (AA-P↓) calculated by PBE is 0.73 eV (0.07 eV), and that calculated by HSE06 is 1.13 eV (0.16 eV). Due to the band gap change, the transmission functions in both the AA-P↑ and AA-P↓ cases will change to some extent quantitatively. However, since the much big difference in the band gaps of the two polarization states and the very small magnitude in the gap or nearly metallic feature of the AA-P↓, have not changed, the main conclusion will be the same, namely, a large TER ratio will still be achieved.

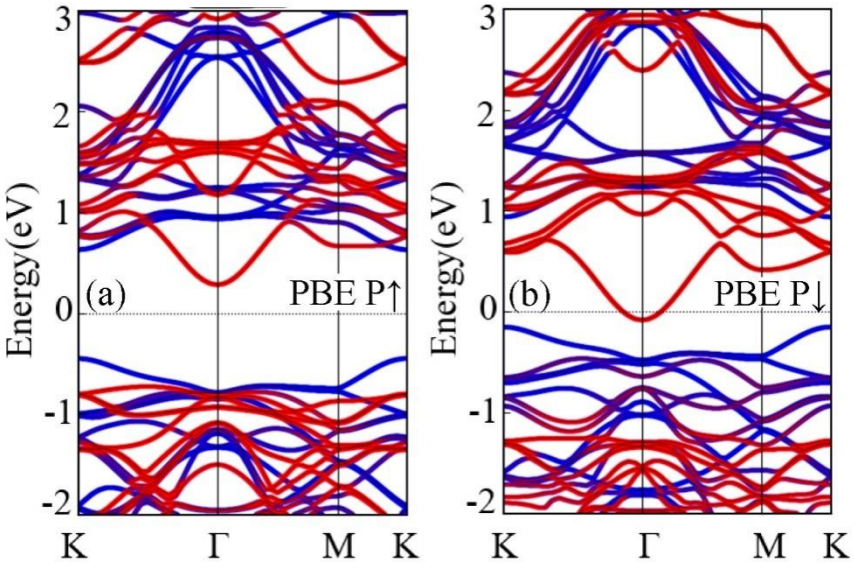

Fig. S1. The band structures of (a) AA-P↑ and (b) AA-P↓ calculated by PBE. In these band structures, the red bands represent the contribution of α-In_2Se_3, while the blue

bands represent the contribution of $MoTe_2$.

S2. The band structures of AA-P↑ and AA-P↓ with SOC.

As can be seen from Fig. S2, the band gap of AA-P↑ with SOC decreases to 0.86 eV (1.03 eV without SOC, see Fig. 3(c)) and the band gap of AA-P↓ with SOC decreases to 0.03 eV (0.16 eV without SOC, see Fig. 3(d)). So the band gaps of AA-P↑ and AA-P↓ with SOC decrease because of the decrease of the band gap of $MoTe_2$ monolayer with SOC. However, AA-P↑ is still a semiconductor with a large band gap and AA-P↓ still owns small band gap and its CB crosses E_F.

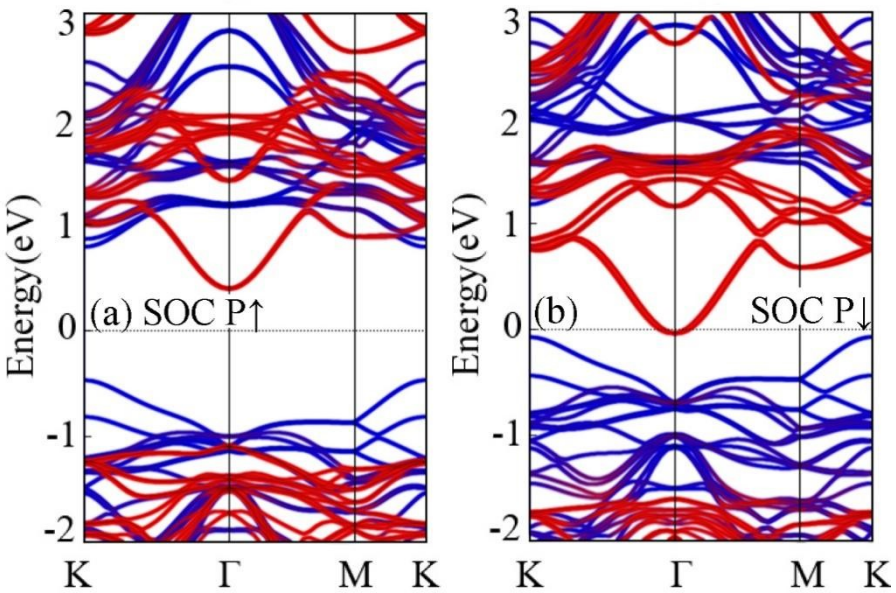

Fig. S2. The band structures of (a) AA-P↑ and (b) AA-P↓ with SOC. The red bands represent the contribution of α-In_2Se_3, while the blue bands represent the contribution of $MoTe_2$.