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

Electronic Supplementary Information

I. THE STACKING SEQUENCES OF THE COMPONENTS HAS NO EFFECT ON THE THERMOELECTRIC PERFORMANCE OF HETEROJUNCTION

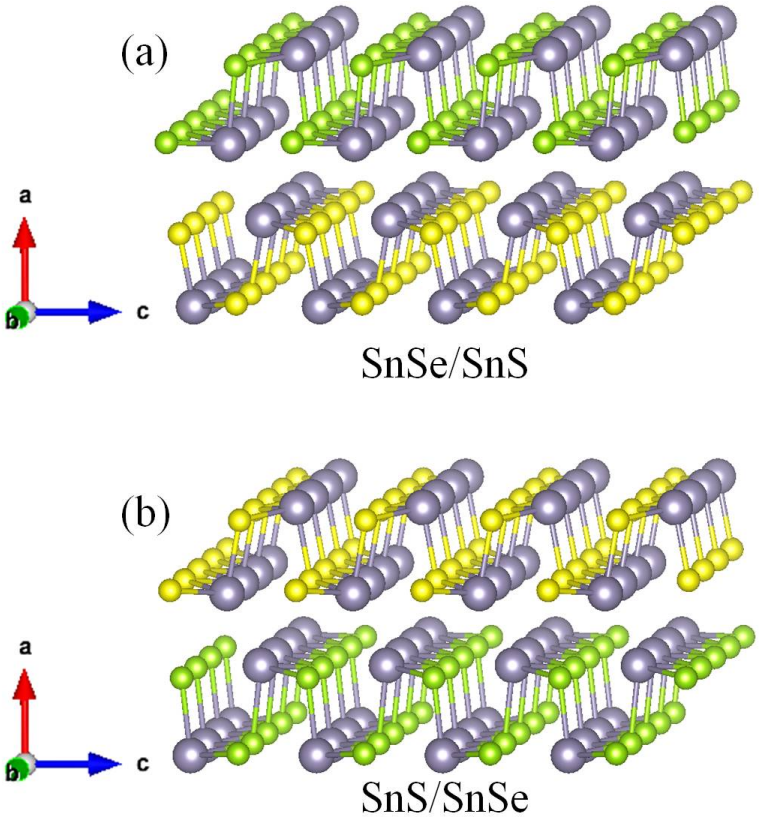

FIG. S1. The atomic structures of (a) heterojunction SnSe/SnS (monolayer SnSe on top) and (b) heterojunction SnS/SnSe (monolayer SnSe on bottom). The gray, green and yellow balls represent tin, selenium and sulfur atoms, respectively.

The atomic structures of heterojunction SnSe/SnS (monolayer SnSe on top) and heterojunction SnS/SnSe (monolayer SnSe on bottom) are shown in Fig. S1 (a) and (b). Both SnSe/SnS and SnS/SnSe are composed of monolayer SnSe and monolayer SnS through van der Waals forces. The only difference between the two structures is that their stacking sequence of components is different. Theoretically, SnSe/SnS could be obtained by flipping SnS/SnSe 180 degrees, the two structures are exactly the same structure as shown in Fig. S1. In fact, the calculated lattice constants of the two structures are exactly the same (b = 4.14 Åand c = 4.45 Å), which is consistent with our previous analysis. In order to further verify our conclusion, we simply calculated the band structures of the two structures, as shown in Fig. S2. It is found that the band gap values of the two structures are exactly the same, and the band structures (especially at the bottom of the conduction band and the top of the valence band) are basically the same, indicating the two structures have the same crystal structure. Based on these, we believe that the two structures are equivalent. More specifically, the stacking sequences has no effect on the thermoelectric performance of heterojunction.

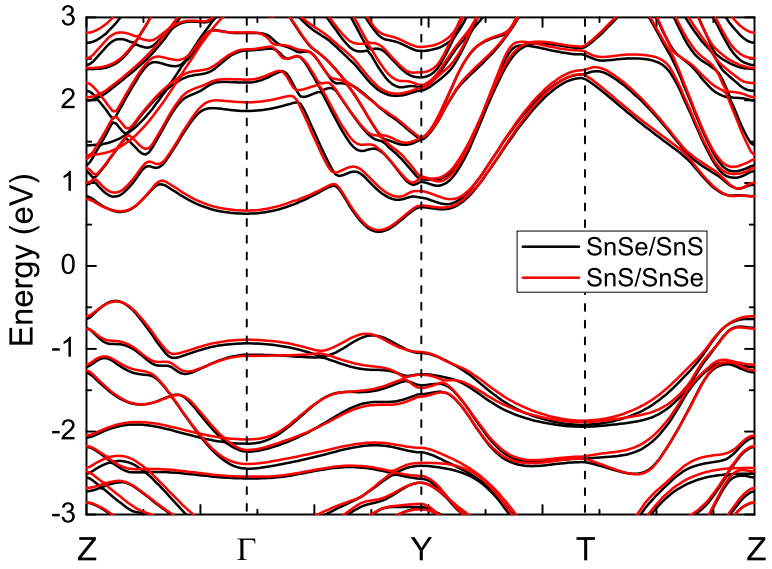

FIG. S2. The band structures of heterojunctions SnSe/SnS and SnS/SnSe. The Fermi energy is set to 0 eV.