Supplementary Information for

The electronic transport properties of transition-metal dichalcogenides lateral heterojunctions

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1 Geometrical structures optimization

We first optimize the unit cell of MoS_2, WS_2, MoS_2–WS_2ud, and WS_2–MoS_2ud by LBFGS method. The k-points grid 1 × 1 × 51 is used to sample the Brillouin zone of the unit cell in the X, Y, and Z direction (periodic direction), respectively. The convergence criterion is that the absolute value of force acting on each atom is less than 0.01 eV/Å.

The two-probe structures can be obtained directly from their optimized unit cell for MoS_2, WS_2, MoS_2–WS_2ud, and WS_2–MoS_2ud nanojunctions. While for MoS_2-WS_2lr, MoS_2\$WS_2$, and MoS_2/WS_2 nanojunctions, we first obtained their relaxed structures by Bulk Rigid Relaxation (BRR) method. Namely, we extract the central scattering region bulk and relax it with "Rigid" constraints on the atoms belonging to the electrode extensions. These MoS_2-WS_2lr, MoS_2\$WS_2$, and MoS_2/WS_2 nanojunctions are then reassembled from the relaxed bulk. This is a computationally efficient approach and will usually capture a large fraction of the required geometry relaxation.

2 Width effect

The WS_2–MoS_2ud lateral heterojunctions with finite width (6, 8, and 10 zigzag chains) have very similar band structures and *I–V* curves, as shown in Fig. S1. The ribbon width palys little influence on their electronic transport properties.

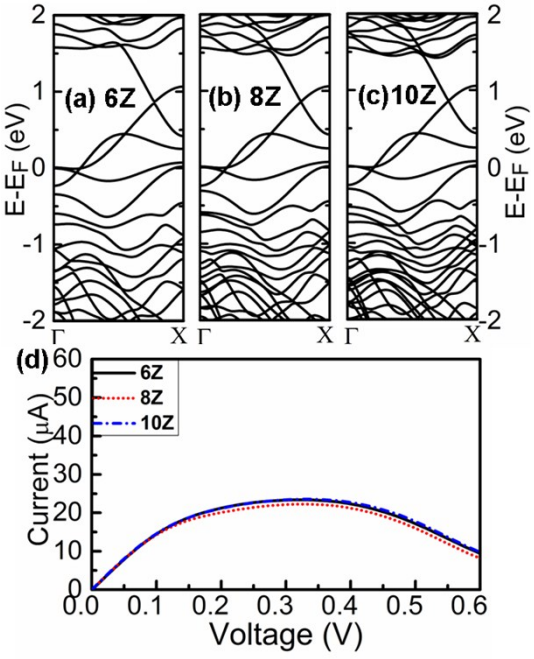

Fig. S1 (a)-(c) refer to the band structures of WS_2–MoS_2ud with 6, 8, and 10 zigzag chains. (d) refers to their almost coincided *I–V* curves.

3 The length of central scattering region

In the present work, the length of the central scattering region is about 25.3 Å, which plays little influence on the electronic transport of such MoS_2–WS_2 lateral heterojunctions. Take WS_2–MoS_2ud lateral heterojunctions as an example, when the length of central scattering region is increased to 31.6 and 37.9 Å, their *I*–*V* curves are almost coincided, as shown in Fig. S2.

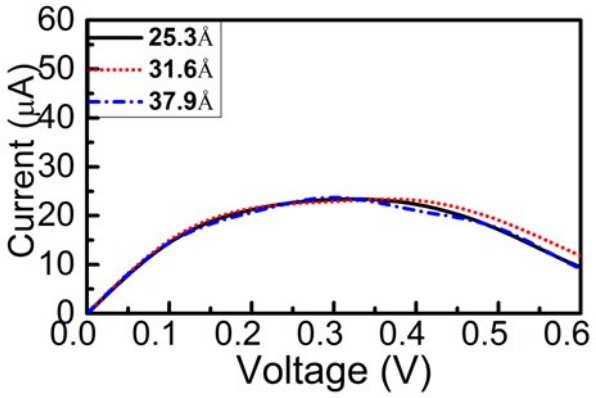

Fig. S2. The *I*–*V* curves of WS_2–MoS_2ud heterojunctions with different lengths for the central scattering region.

4 The eigenstates of MoS_2-WS_2lr and MoS_2–WS_2ud heterojunction

Although these MoS_2–WS_2 lateral heterojunctions have different interfaces, they have the very similar transmission eigenstates distributions. As shown in Fig. S3, the transmission eigesntates of MoS_2-WS_2lr and MoS_2–WS_2ud heterojunctions are the same to that of WS_2–MoS_2ud heterojunction (see Fig. 5 of the paper).

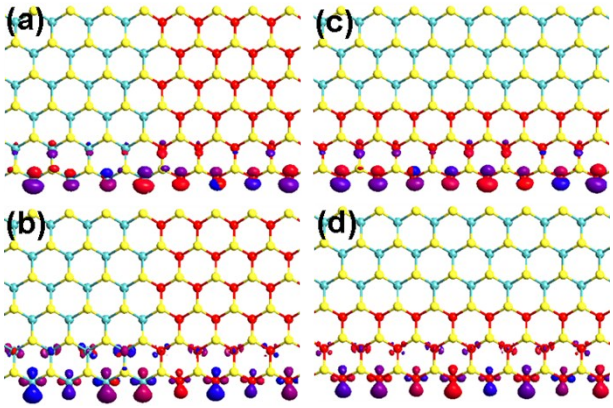

Fig. S3. (a) and (b) refer to the both transmission eigenstates of the MoS_2-WS_2lr heterojunction at 0.15 eV under the bias of 0.3 V. (c) and (d) refer to the both transmission eigenstates of the MoS_2–WS_2ud heterojunction at 0.15 eV under the bias of 0.3 V.