Electronic Supplementary Information for

Size dependence in two-dimensional lateral heterostructures of transition metal dichalcogenides

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For armchair (zigzag) boundary, it is one-unit length along *x* (*y*) direction (see Fig. 1a of the manuscript), i.e. 5.51 Å (3.18 Å). While the length along *y* (*x*) direction varies. To better illustrate the size of the supercell employed in this work, we list the length and the number of atoms in Table S1 and S2.

Table S1. The length (as labelled in Fig. 1 of the manuscript) and the number of atoms employed in the supercell along armchair direction.

Length (Å)	Number of atoms
19.1	**36**
38.2	**72**
57.3	**108**
76.4	**144**
114.6	**216**
152.8	**288**
191.0	**360**
229.2	**432**
305.5	**576**

343.7	**648**
458.3	**864**

Table S2. The length (as labelled in Fig. 1 of the manuscript) and the number of atoms employed in the supercell along zigzag direction.

Length (Å)	Number of atoms
44.1	**48**
88.2	**96**
132.3	**144**
176.4	**192**
264.6	**288**
352.8	**384**
441.0	**480**
529.2	**576**
705.6	**768**
882.0	**960**
1058.4	**1152**
1411.2	**1536**
1764.0	**1920**
2116.8	**2304**
2756.3	**3000**
3528.0	**3840**
4233.6	**4608**

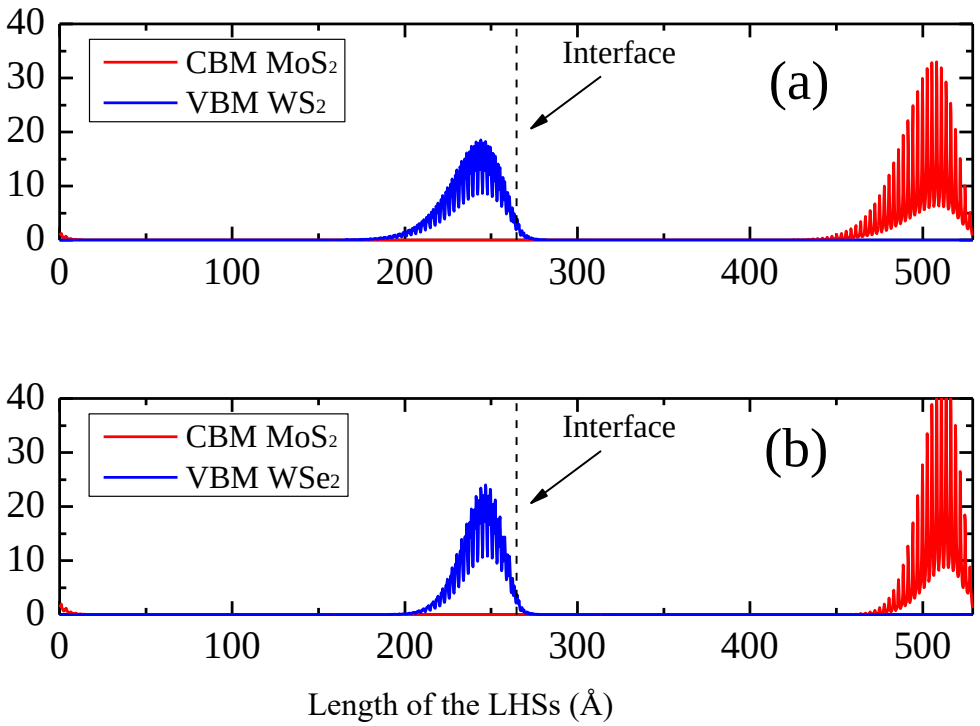

Fig. S1. Plane integrated modular square wave functions of the VBM ($|\psi_v(r)|^2$) and CBM ($|\psi_c(r)|^2$) for (a) MoS_2/WS_2 and (b) MoS_2/WSe_2 LHSs.

As shown in Fig. R1, the plane integrated modular square wave functions of the VBM ($|\psi_v(r)|^2$) and CBM ($|\psi_c(r)|^2$) of the MoS_2/WSe_2 LHS are similar to those of MoS_2/WS_2 LHS. As have been discussed in the manuscript, those wave functions determine the band structures of the LHSs. As such, we believe that MoS_2/WSe_2 LHS can show similar trend as compared with MoS_2/WS_2 LHS. Consequently, our conclusions are not limited to MoS_2/WS_2 LHS, but can be applied to other TMDs LHSs.