Electronic Supplementary Information for

Enhanced photoelectric performance of MoSSe/MoS_2 van der Waals heterostructure with tunable multiple band alignments

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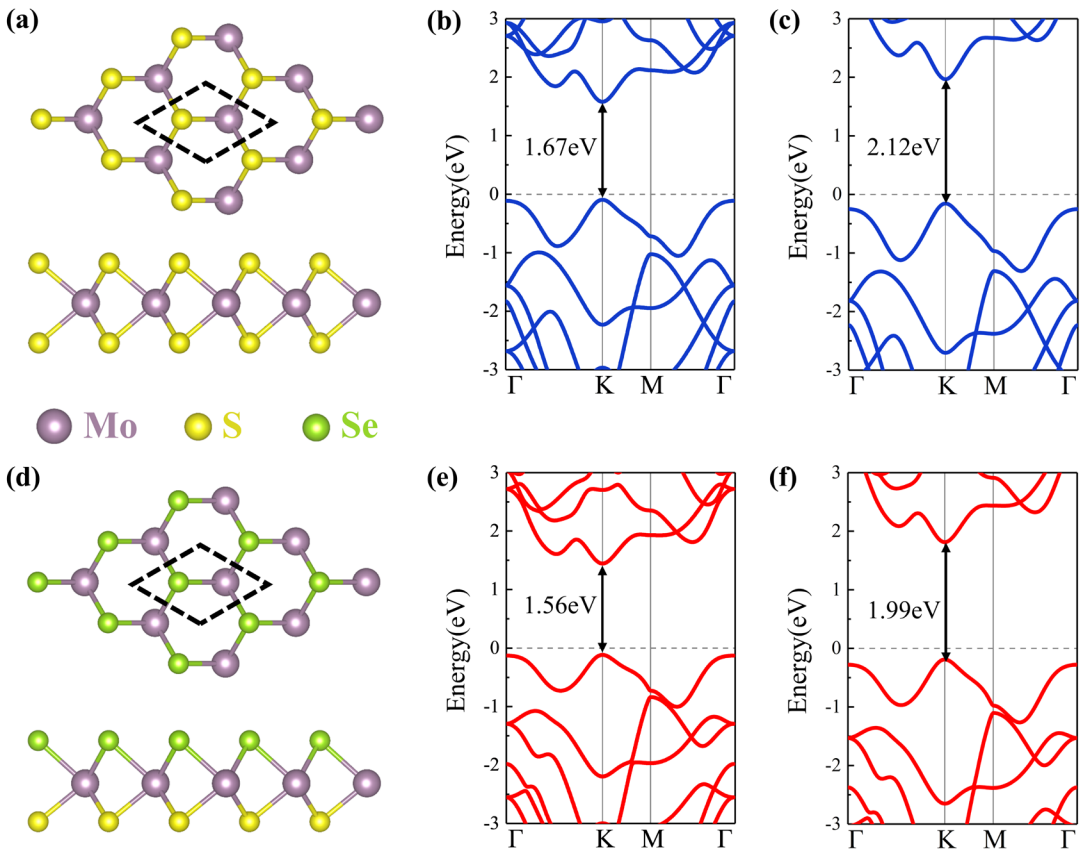

Fig. S1 Top and side views of (a) MoS_2 and (d) MoSSe monolayers. The lavender, yellow and green beads represent Mo, S, and Se atoms, respectively. The black dashed rhombuses mark the unit cells. Calculated band structures of (b and c) MoS_2 and (e and f) MoSSe monolayers based on PBE and HSE, respectively. The Fermi level is set to 0 eV.

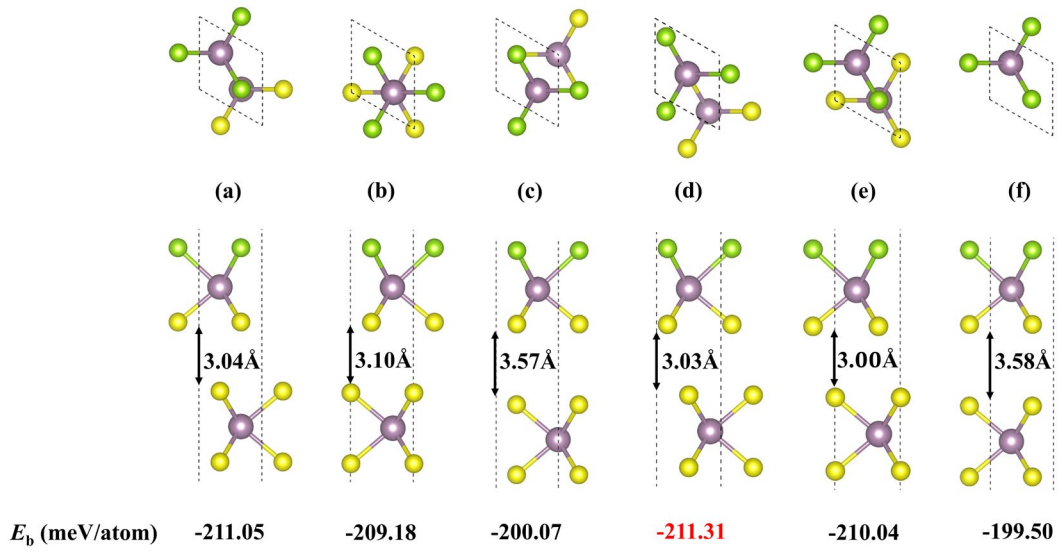

Fig. S2 Top and side views of high symmetry stacking model of (a) AB, (b) A'B , (c) AB', (d) AA, (e) A'A, and (f) AA' for the MoSSe/MoS_2(I) vdWH. The interlayer distance and the binding energy (E_b) are labeled.

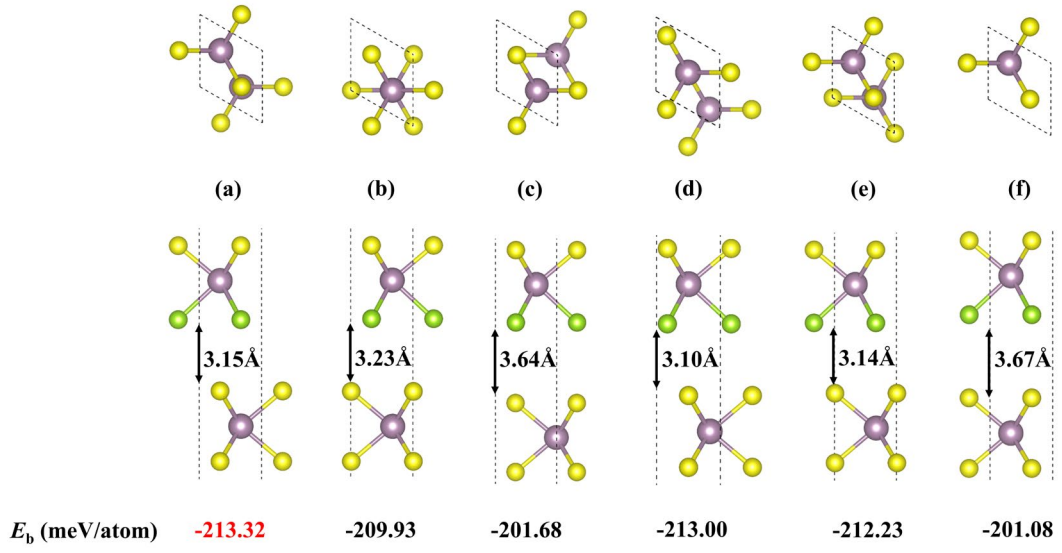

Fig. S3 Top and side views of high symmetry stacking model of (a) AB, (b) A'B , (c) AB', (d) AA, (e) A'A, and (f) AA' for the MoSSe/MoS_2(II) vdWH. The interlayer distance and the binding energy (E_b) are labeled.

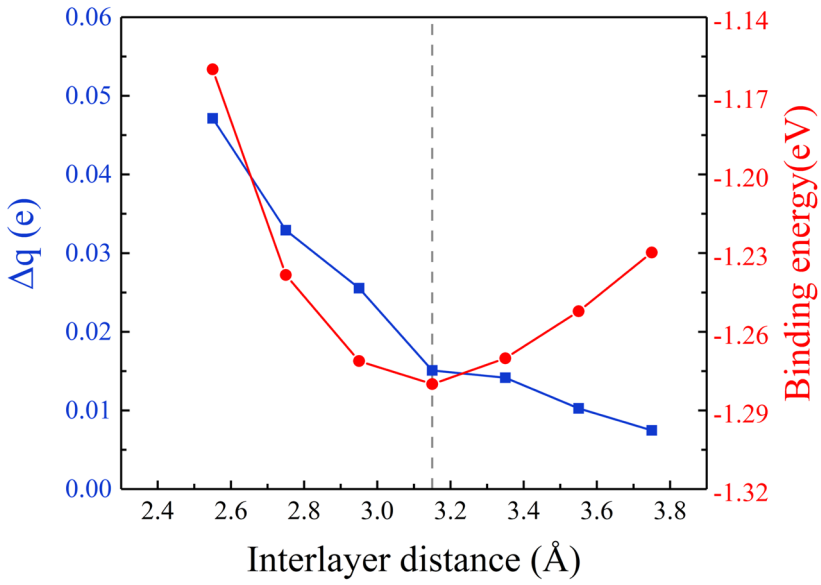

Fig. S4 Variation of binding energy and charge transfer with interlayer distance for the MoSSe/MoS_2(II) vdWH.