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Supporting Information

Characteristics of lateral and hybrid heterostructures based on monolayer MoS_2: A computational study

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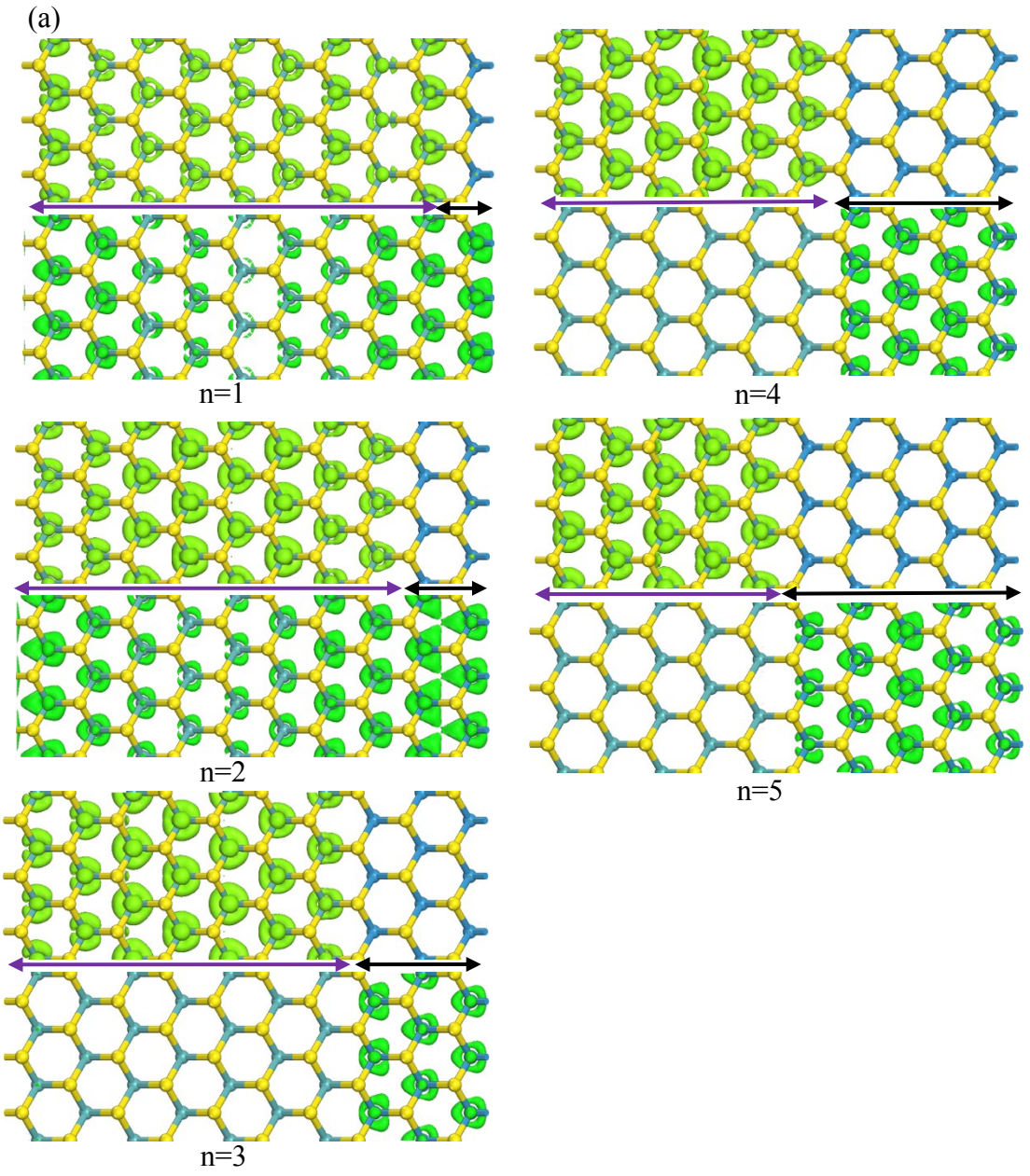

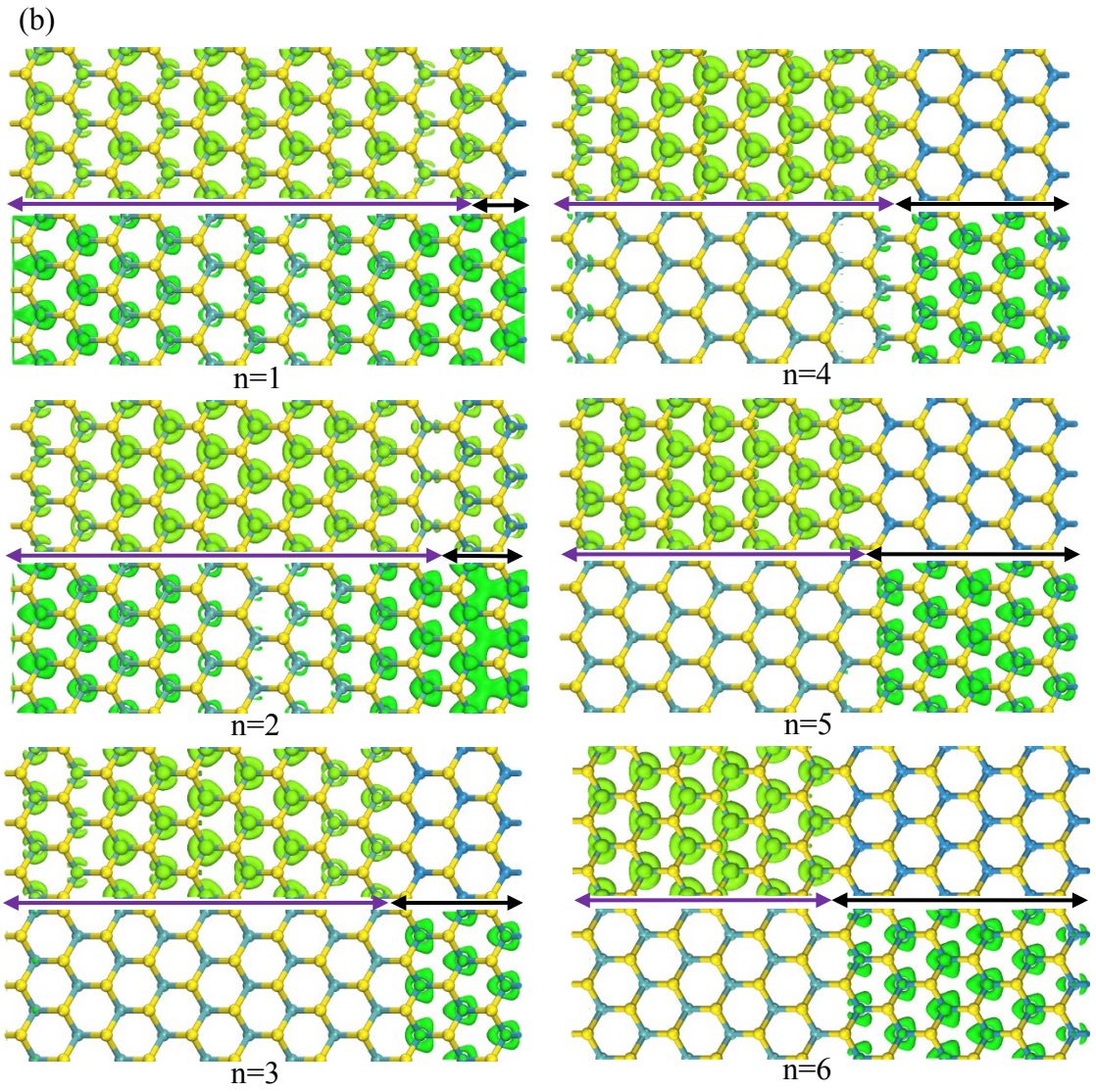

Figure S1. $MoS_2/(WS_2)_n$ lateral heterostructure as an example to illustrate the charge distribution of $MoS_2(MX_2)_n$ lateral heterostructure dependent of the size of heterostructure. (a) and (b) show the charge density of CBM and VBM states in $[MoS_2/(WS_2)_n]_{10}$ and $[MoS_2/(WS_2)_n]_{12}$ lateral heterostructures, respectively. The up side panels are charge density of CBM. The below side panels are charge density of VBM.

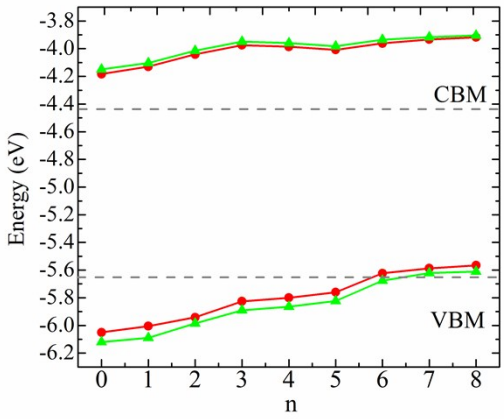

Figure S2. Evolution of band edges of the $MoS_2/(MoSe_2)_n$ lateral heterostructures as a function of the width n of $MoSe_2$ region. The green and red lines stand for the results calculated by HSE06 and GGA functionals, respectively. The up and low gray dash line represent the water reduction and oxidation potential levels, respectively.

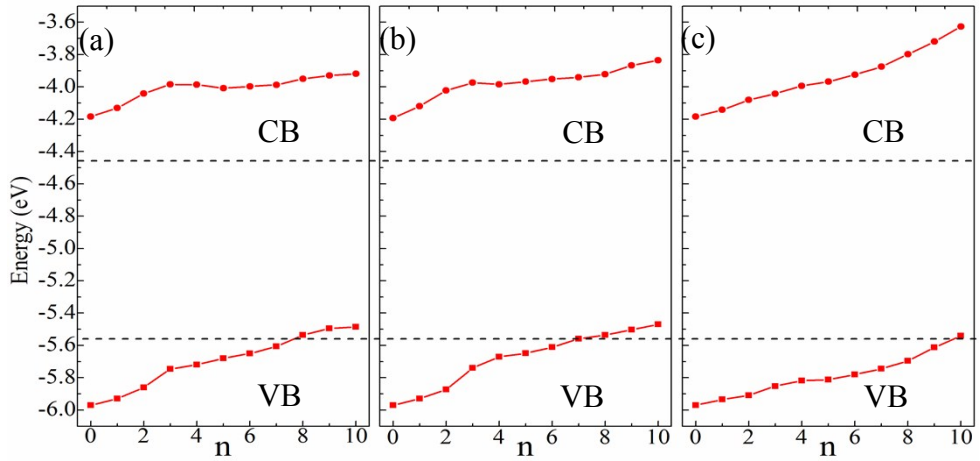

Figure S3. The band edges of $MoS_2/(MoSe_2)_n$, $MoS_2/(WSe_2)_n$, and $MoS_2/(WS_2)_n$ lateral heterostructures as a function of the width n (a-c). These lateral heterostructures contain ten lines transition metal. The dash lines represent the water oxidation and reduction potentials levels, respectively.

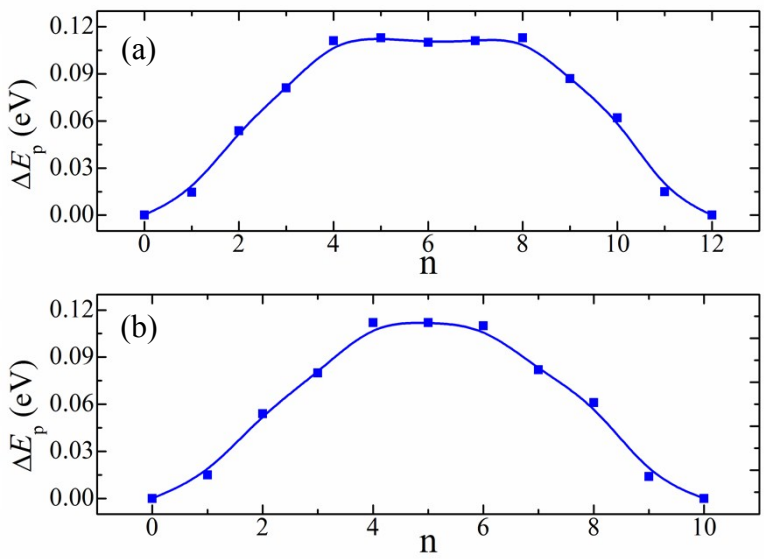

Figure S4. The electrostatic potential barriers of lateral heterostructures (a) $[MoS_2/(WS_2)_n]_{10}$ and (b) $[MoS_2/(WS_2)_n]_{12}$ various for the width n of WS_2.