Effect of Doping and Defects on the Electronic Properties of MoS$_2$/WSe$_2$ Bilayer Heterostructure: A First-principles Study

Xingliang Wang, [a] Guijuan Zhao,*[a] Xiurui Lv, [a] Mingyang Zhao, [b] Wanting Wei [a] and Guipeng Liu [a]

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Supplementary Materials

Table S1 The lattice constants, interlayer distance, and formation energy for the four configurations using DFT-D3(BJ).

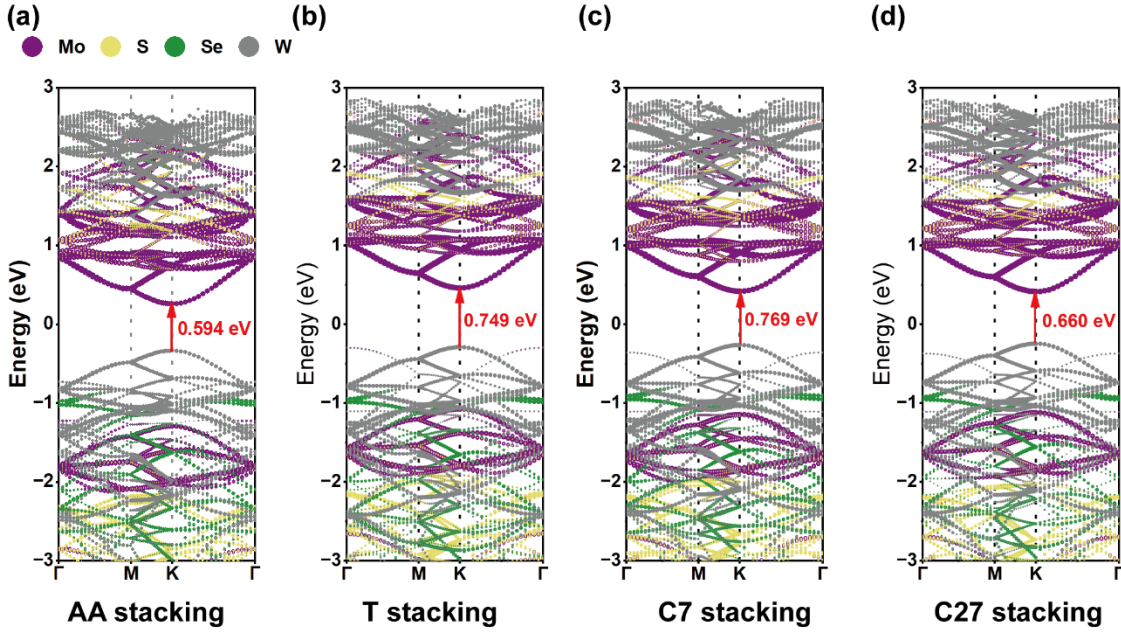| Stacking	a(Å)	Interlayer distance (Å)	Formation Energy (eV)	Bandgap (eV)
AA	3.214	3.579	-1.984	0.594
T	3.216	2.925	-3.659	0.749
C7	3.226	2.968	-3.618	0.769
C27	3.218	3.036	-3.206	0.660

Fig. S1. The band structure of (a) AA stacking, (b)T stacking, (c) C7 stacking, (d) C27 stacking MoS$_2$/WSe$_2$ bilayer heterostructure using DFT-D3(BJ).
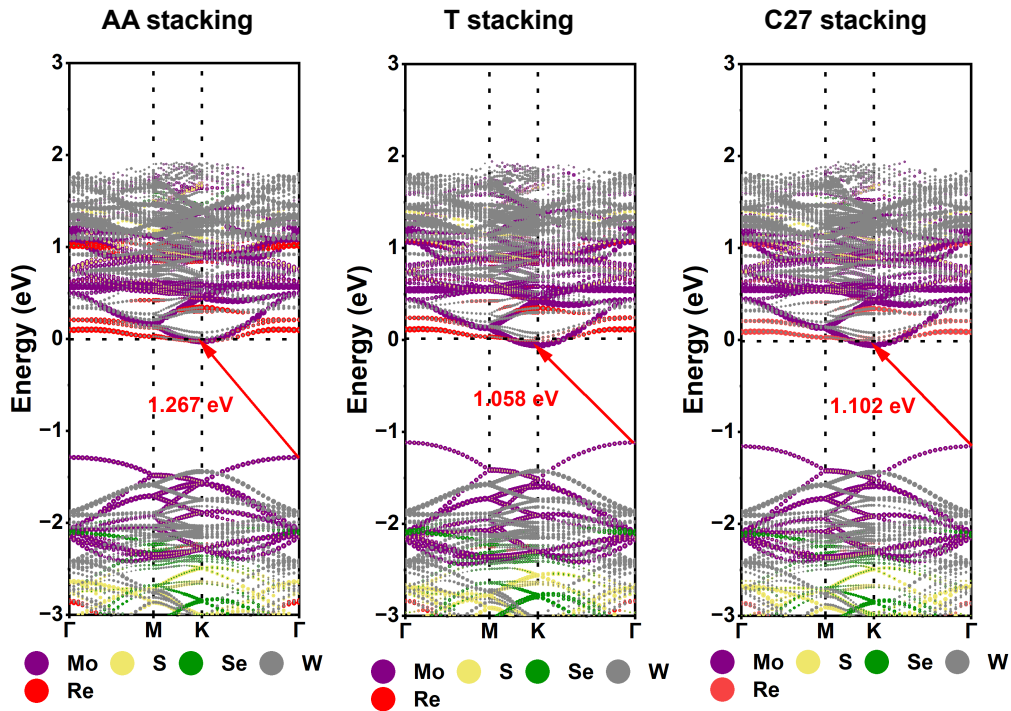

Fig. S2. The band structure of (a) AA stacking, (b)T stacking, and (c) C27 stacking MoS$_2$/Re-doped WSe$_2$ bilayer heterostructures.

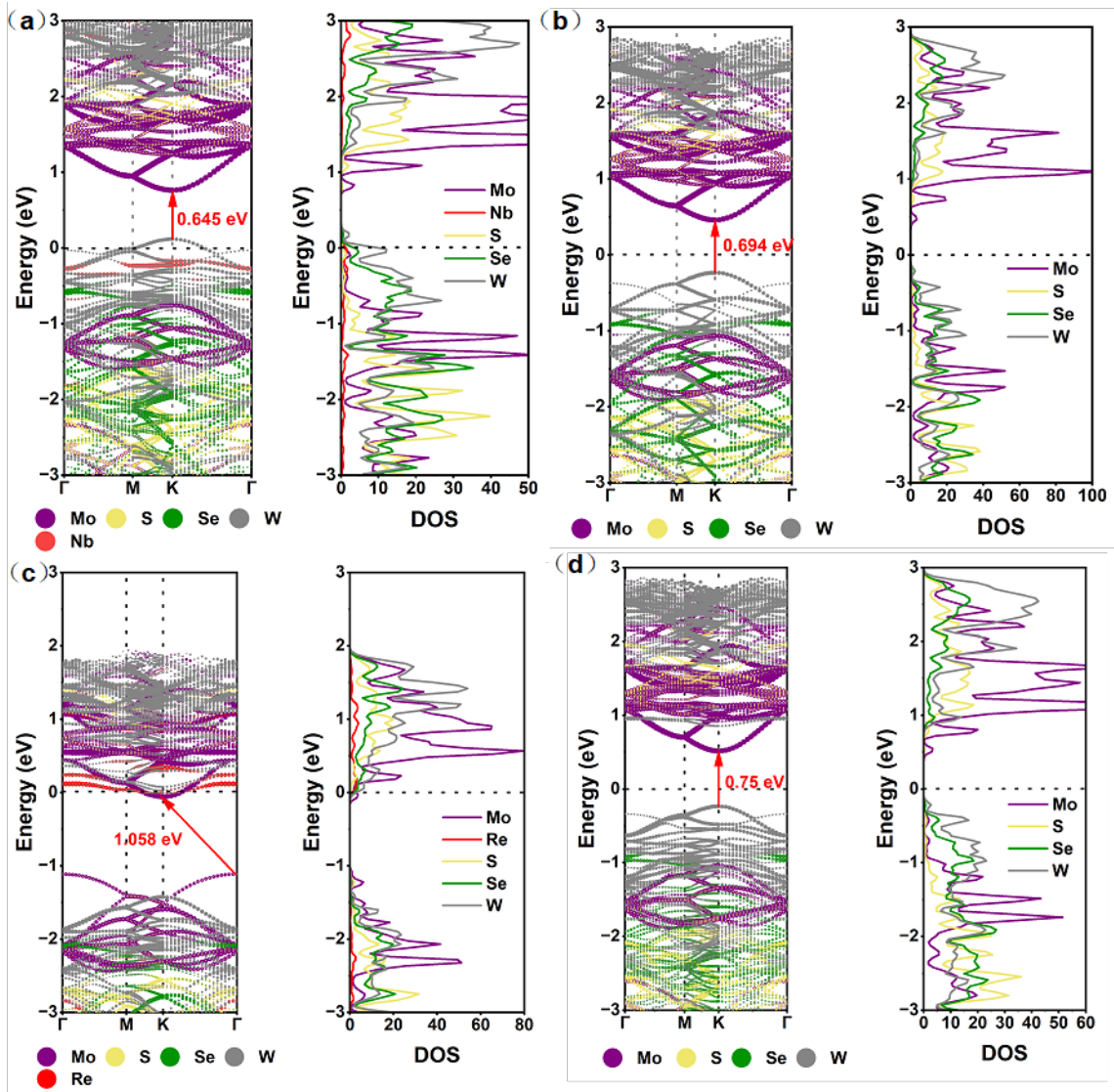Fig. S3. The band structure and DOS of (a) MoS_2/Nb-doped WSe_2 bilayer heterostructure, (b) MoS_2/Mo-doped WSe_2 bilayer heterostructure, (c) MoS_2/Re-doped WSe_2 bilayer heterostructure, and (d) MoS_2/Se-vacancy WSe_2 bilayer heterostructure under T stacking.