



Supplementary Materials

Tunable Electronic Properties of Lateral Monolayer Transition Metal Dichalcogenide Superlattice Nanoribbons

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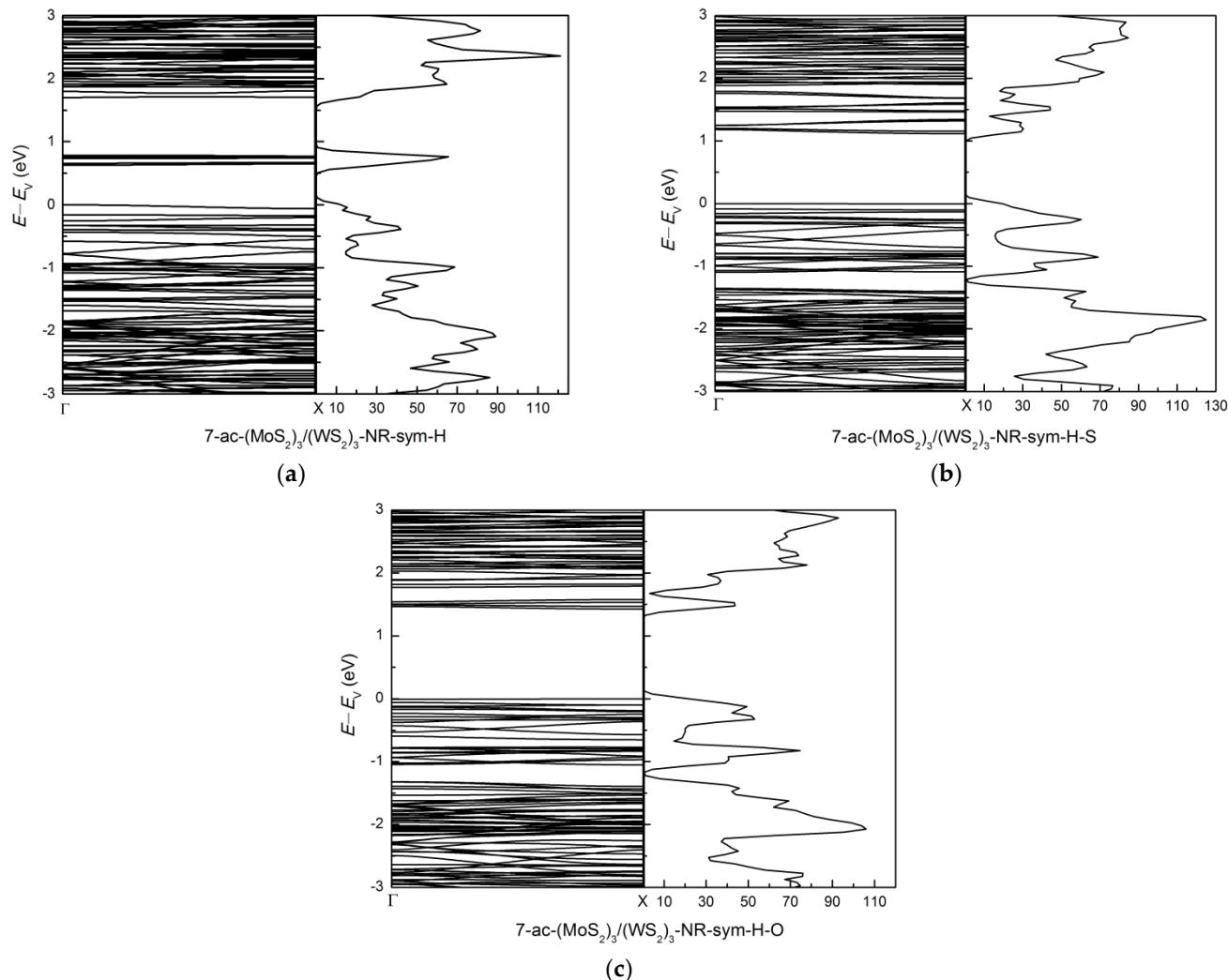


Figure S1. The band structure and dos: (a) 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H, (b) 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H-S and (c) 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H-O.

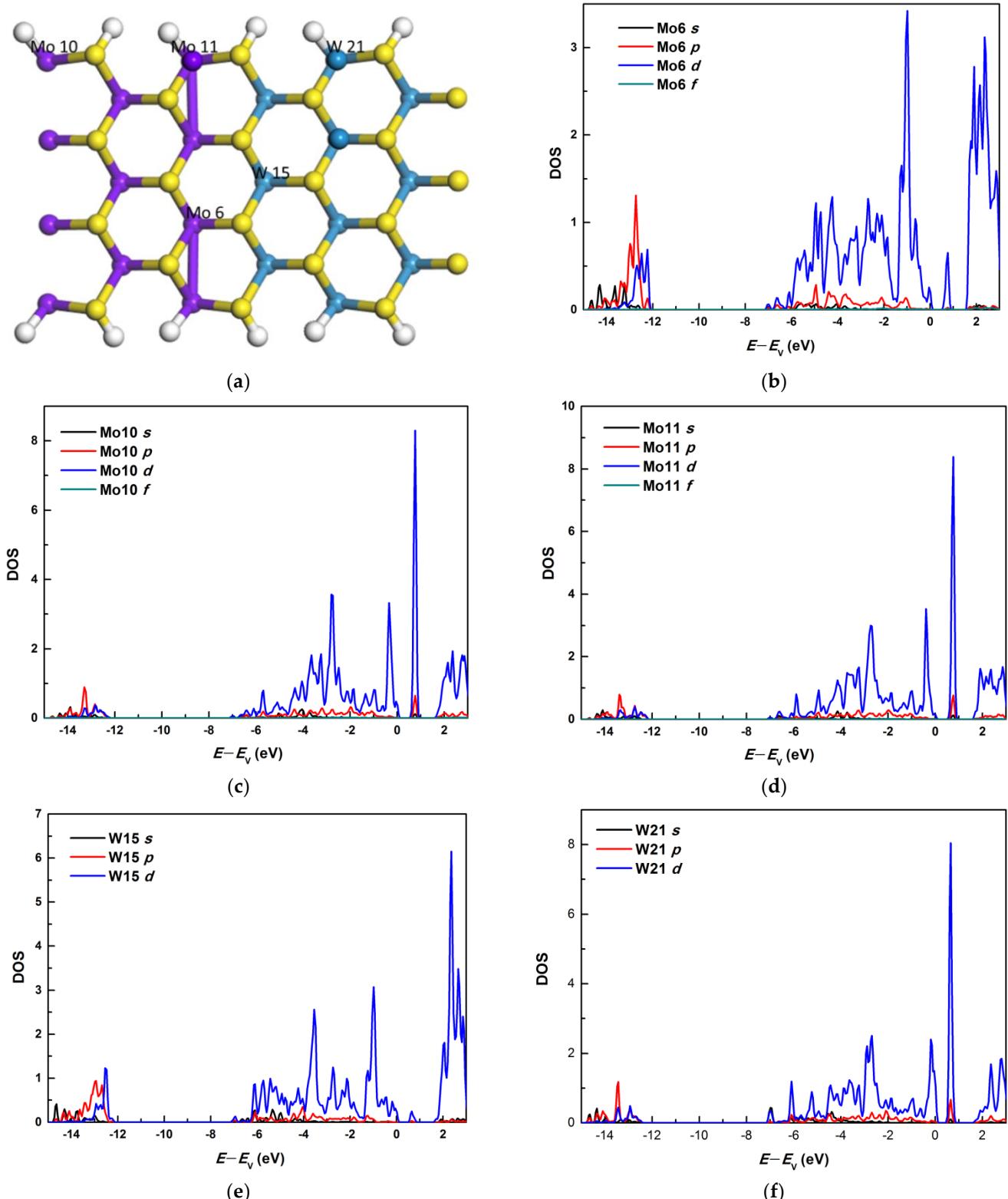


Figure S2. (a) The relaxed geometry of 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H, edge and inside atoms for Mo and W are labeled. The partial density of states (pdos) for (b) inside Mo6 atom; (c) edge Mo10 atom; (d) edge Mo11 atom; (e) inside W15 atom; (f) edge W21 atom of 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H nanoribbon.

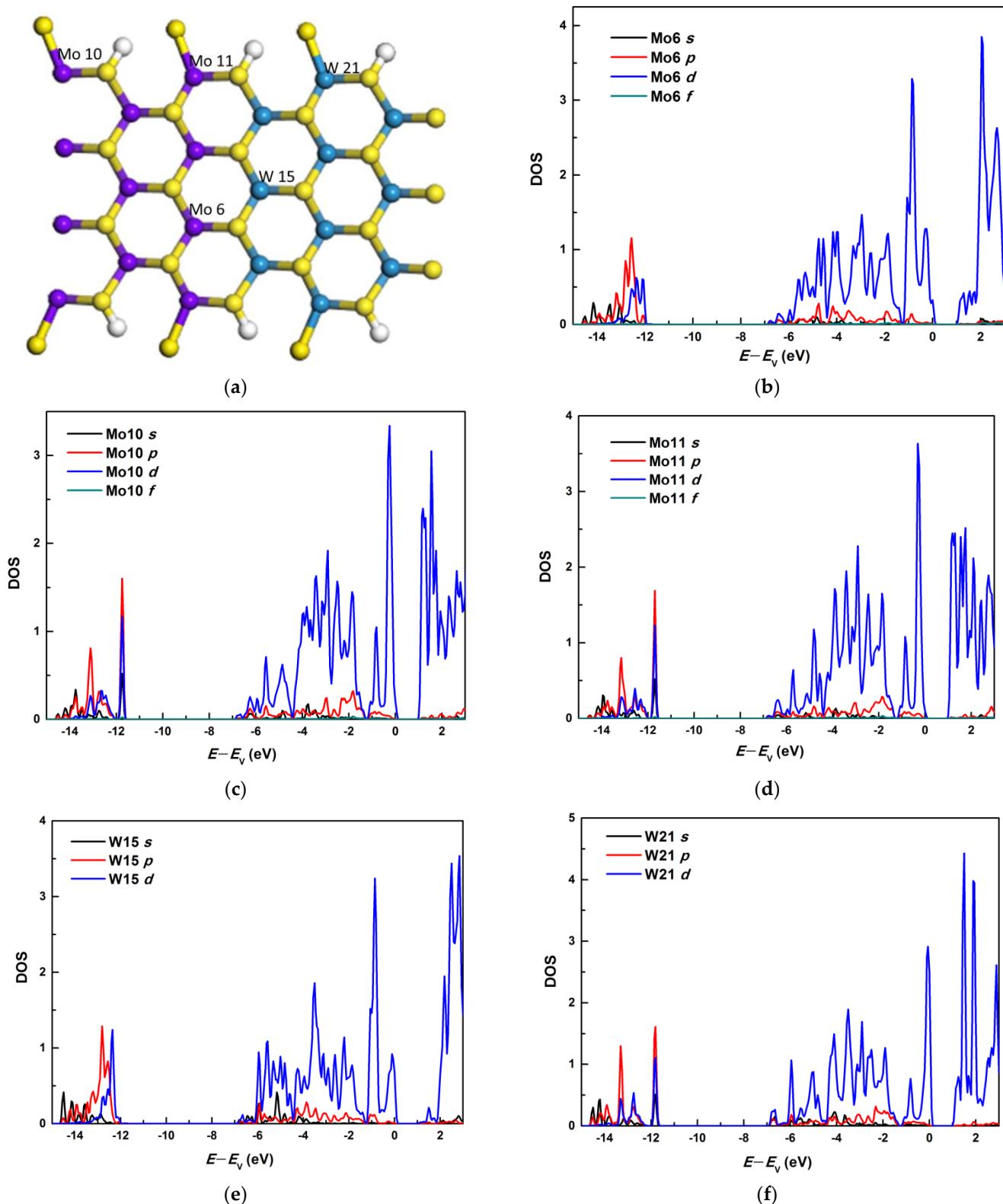


Figure S3. (a) The relaxed geometry of 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H-S, edge and inside atoms for Mo and W are labeled. The partial density of states (pdos) for (b) inside Mo6 atom; (c) edge Mo10 atom; (d) edge Mo11 atom; (e) inside W15 atom; (f) edge W21 atom of 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H-S nanoribbon.

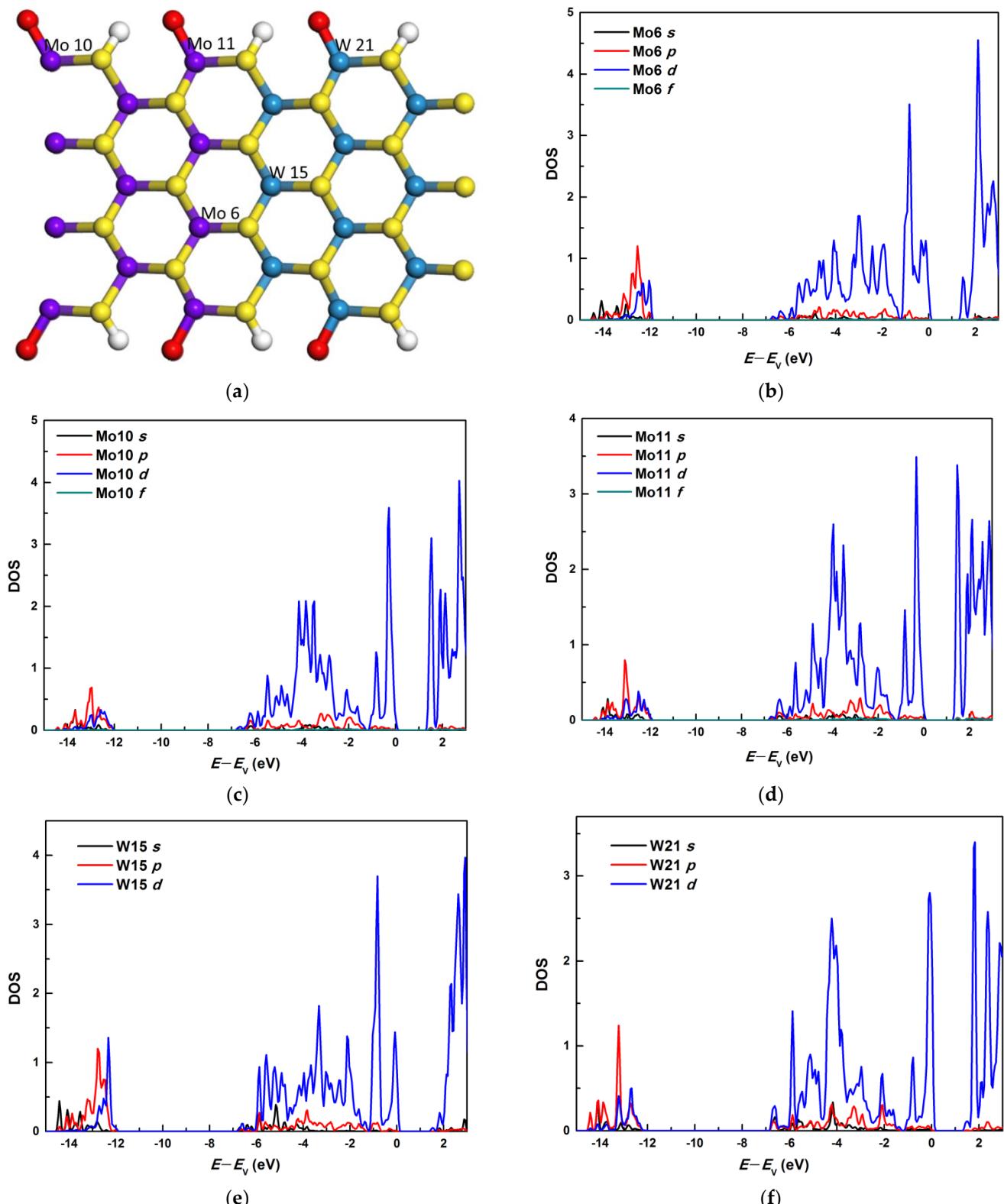


Figure S4. (a) The relaxed geometry of 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H-O, edge and inside atoms for Mo and W are labeled. The partial density of states (pdos) for (b) inside Mo6 atom; (c) edge Mo10 atom; (d) edge Mo11 atom; (e) inside W15 atom; (f) edge W21 atom of 7-ac-(MoS₂)₃/(WS₂)₃-NR-sym-H-O nanoribbon.

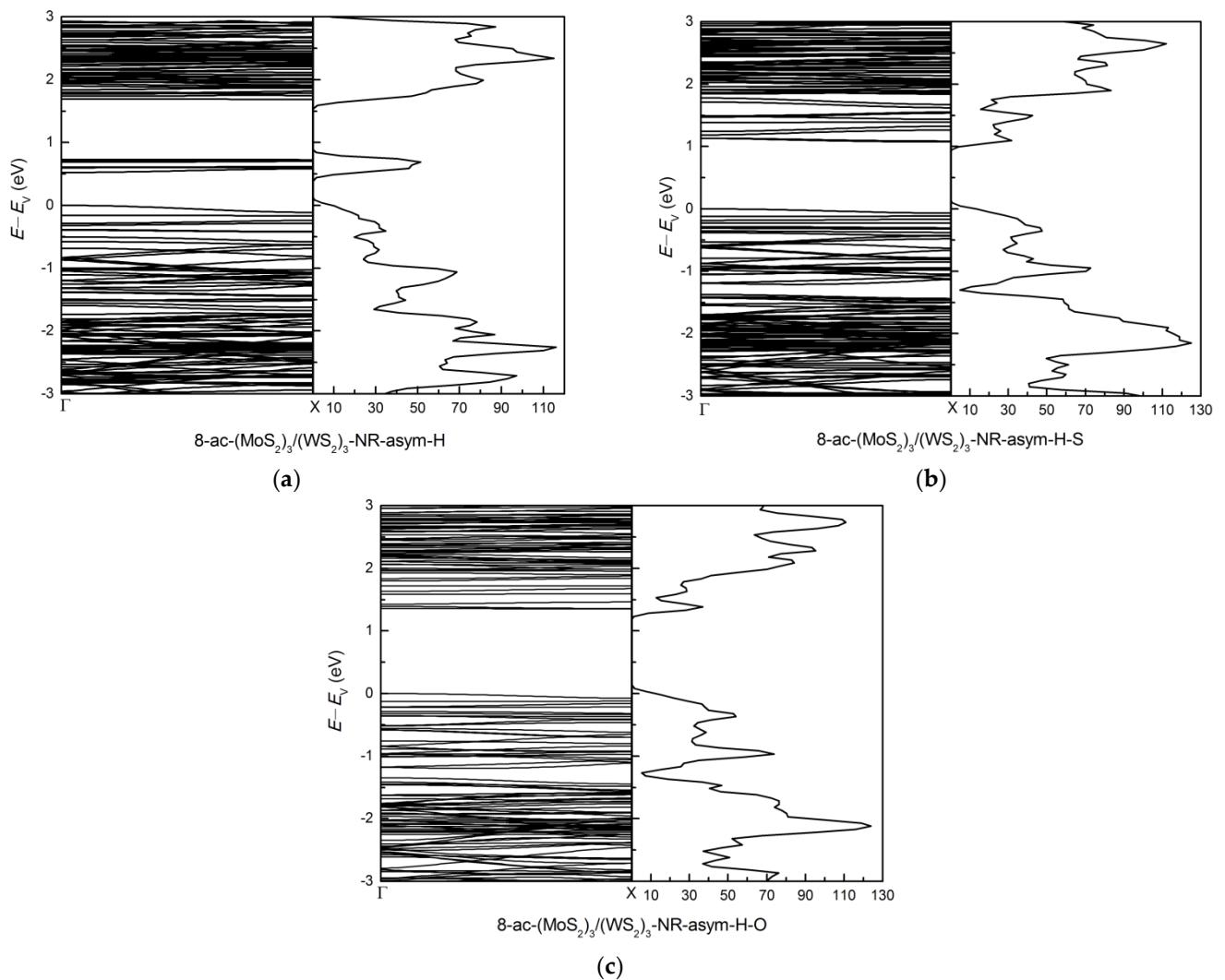


Figure S5. The band structure and dos: (a) 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H, (b) 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H-S and (c) 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H-O.

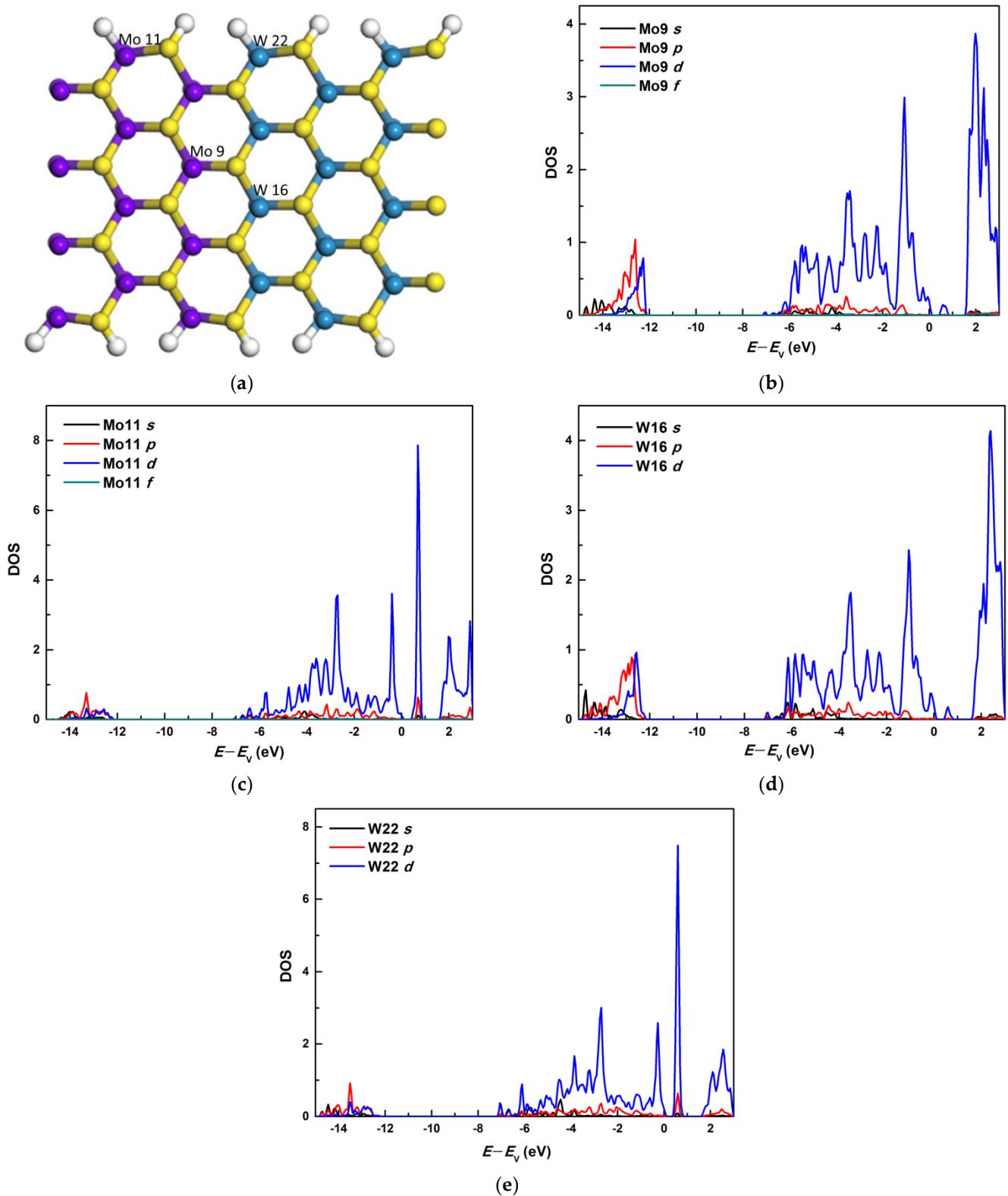


Figure S6. (a) The relaxed geometry of 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H, edge and inside atoms for Mo and W are labeled. The partial density of states (pdos) for (b) inside Mo9 atom; (c) edge Mo11 atom; (d) inside W16 atom; (e) edge W22 atom of 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H nanoribbon.

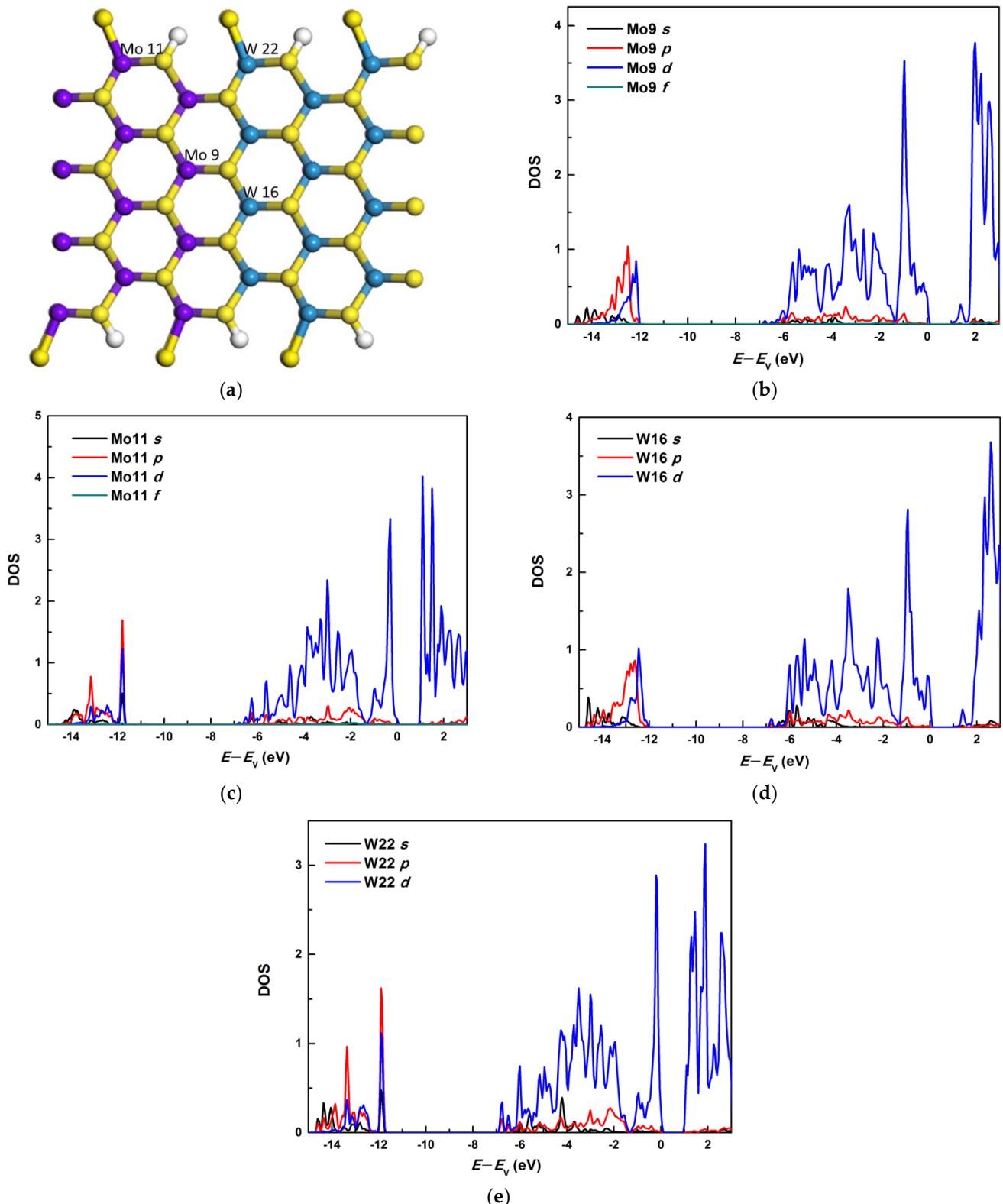


Figure S7. (a) The relaxed geometry of 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H-S, edge and inside atoms for Mo and W are labeled. The partial density of states (pdos) for (b) inside Mo9 atom; (c) edge Mo11 atom; (d) inside W16 atom; (e) edge W22 atom of 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H-S nanoribbon.

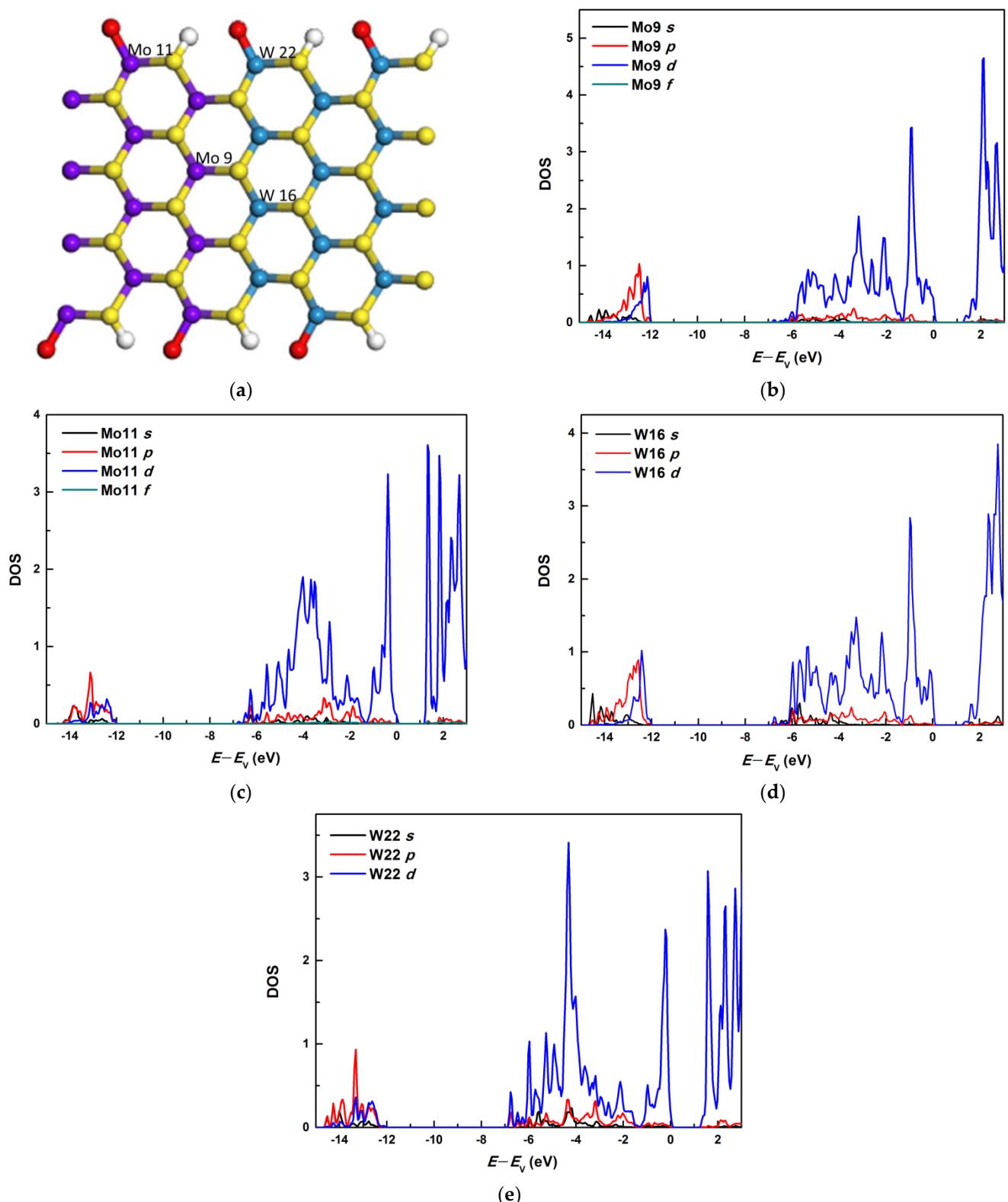


Figure S8. (a) The relaxed geometry of 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H-O, edge and inside atoms for Mo and W are labeled. The partial density of states (pdos) for (b) inside Mo9 atom; (c) edge Mo11 atom; (d) inside W16 atom; (e) edge W22 atom of 8-ac-(MoS₂)₃/(WS₂)₃-NR-asym-H-O nanoribbon.

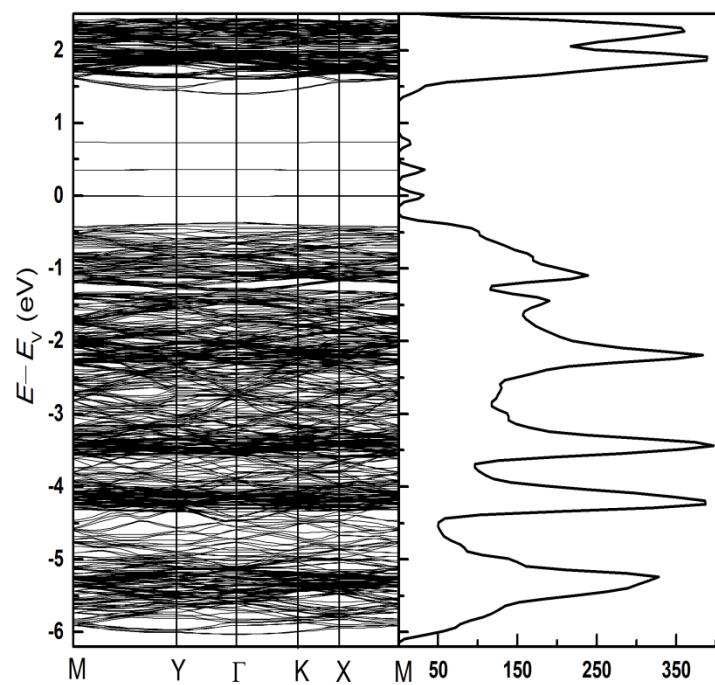
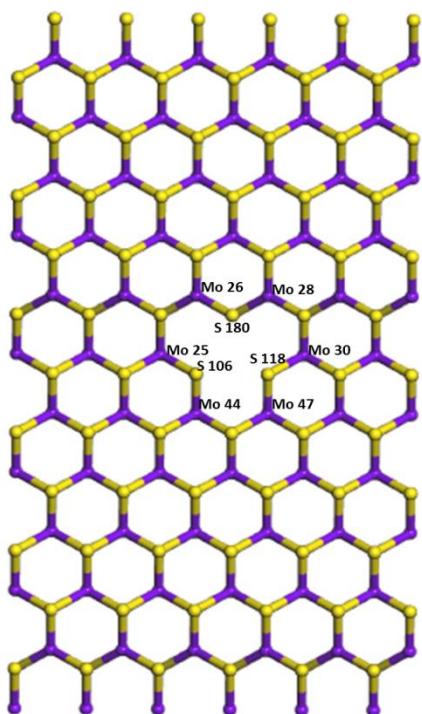
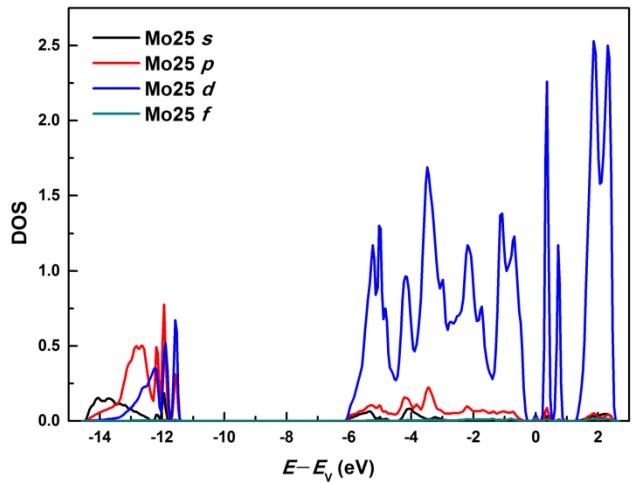


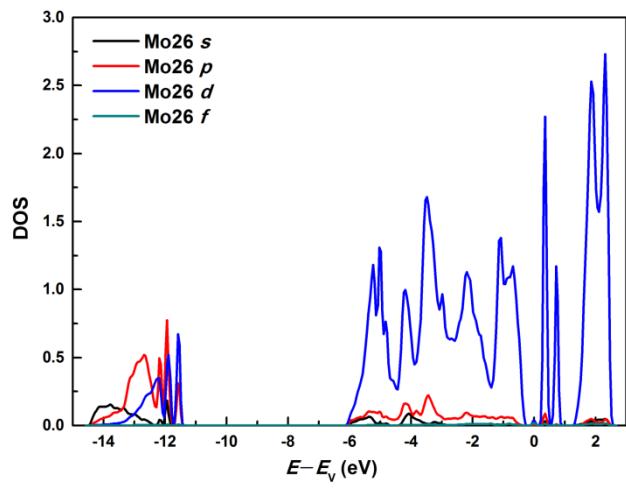
Figure S9. The band structure and dos of MoS₂ SL with a Mo vacancy in the middle.



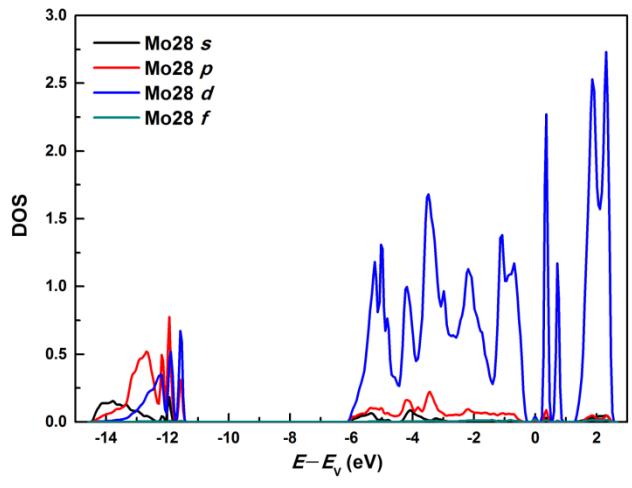
(a)



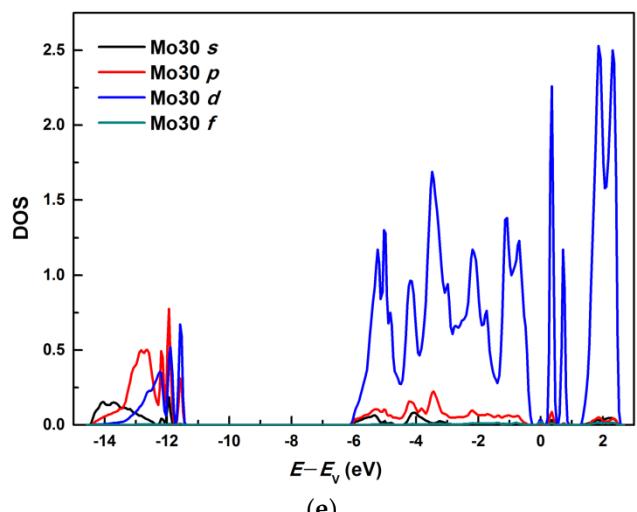
(b)



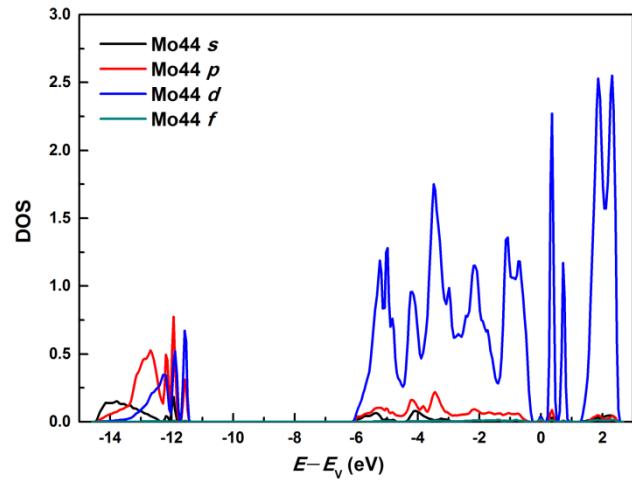
(c)



(d)



(e)



(f)

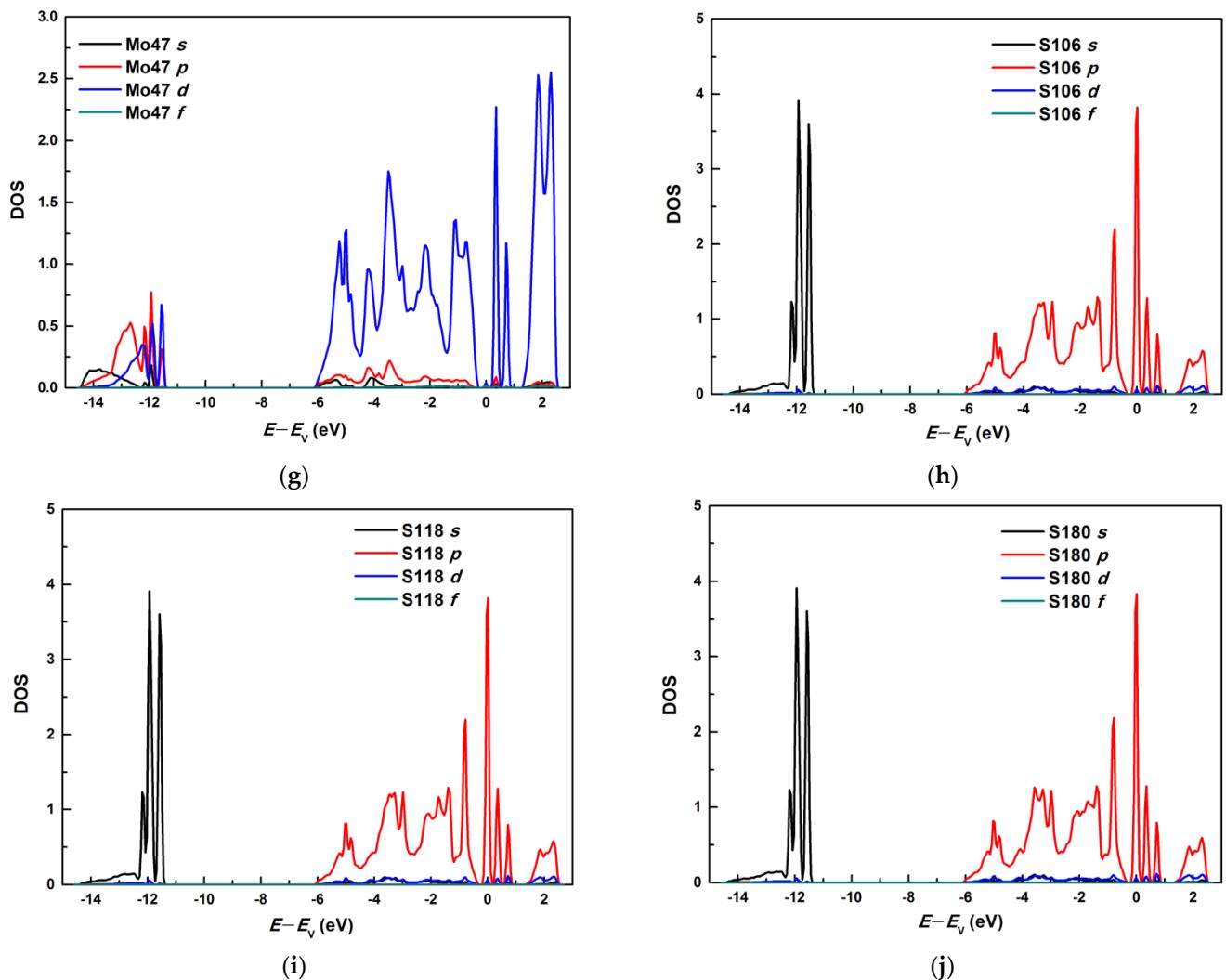


Figure S10. (a)The geometry of MoS₂ SL with a Mo vacancy in the middle and the atoms around Mo vacancy are labeled. The partial density of states (pdos) for atoms around Mo vacancy: (b) Mo25 atom; (c) Mo26 atom; (d) Mo28 atom; (e) Mo30 atom; (f) Mo44 atom; (g) Mo47 atom; (h) S106 atom; (i) S118 atom; (j) S180 atom of MoS₂ SL with a Mo vacancy in the middle.

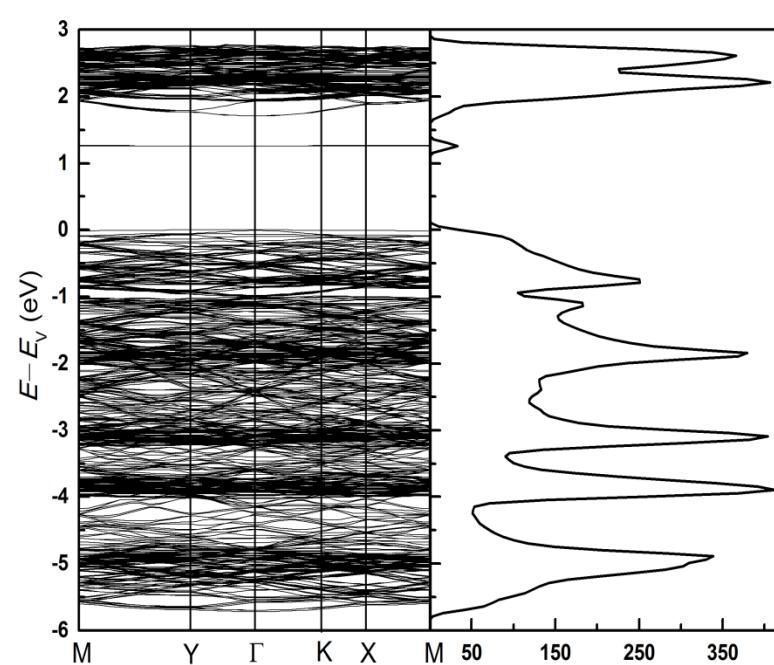


Figure S11. The band structure and dos of MoS₂ SL with a S vacancy in the middle.

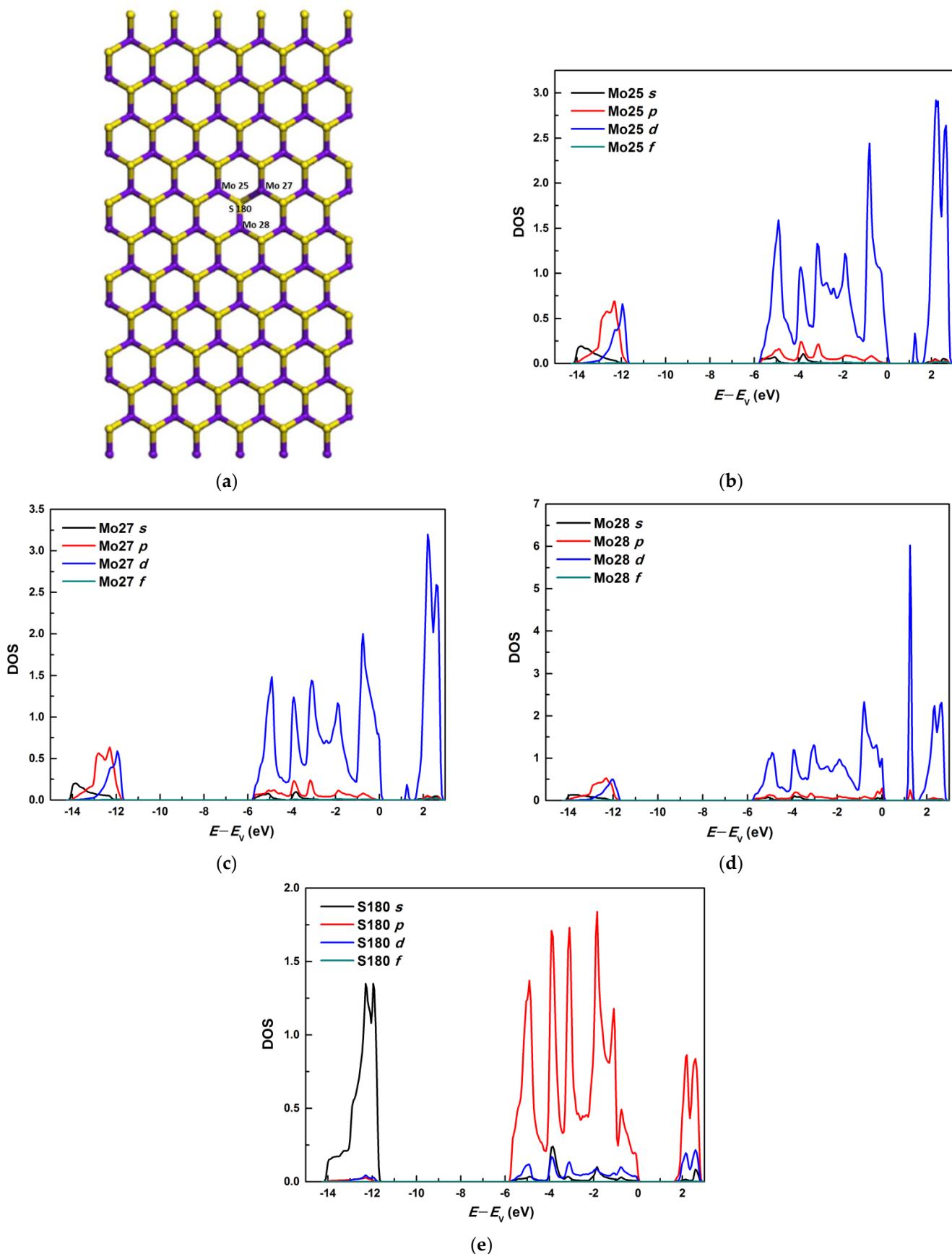


Figure S12. (a) The geometry of MoS₂ SL with a S vacancy in the middle and the atoms around S vacancy are labeled. The partial density of states (pdos) for atoms around S vacancy: (b) Mo25 atom; (c) Mo27 atom; (d) Mo28 atom; (e) S180 atom of MoS₂ SL with a S vacancy in the middle.