S-1, The calculated band structures of MoS$_2$: (a) bulk and (b) monolayer.

S-2, The calculated band structures of zz-MoS$_2$-NR-u: (a) spin-up and (b) spin-down.
S-3, The calculated band structures of H-saturated zz-MoS₂-NR-u: (a) spin-up and (b) spin-down.

S-4, The calculated band structures of zz-MoS₂-NR-Mo-u: (a) spin-up and (b) spin-down.
S-5, The calculated band structures of H-saturated \( \text{zz-MoS}_2\text{-NR-Mo-u} \): (a) spin-up and (b) spin-down.

S-6, The calculated band structures of \( \text{zz-MoS}_2\text{-NR-S-u} \): (a) spin-up and (b) spin-down.
S-7, The calculated band structures of H-saturated zz-MoS$_2$-NR-S-u: (a) spin-up and (b) spin-down.