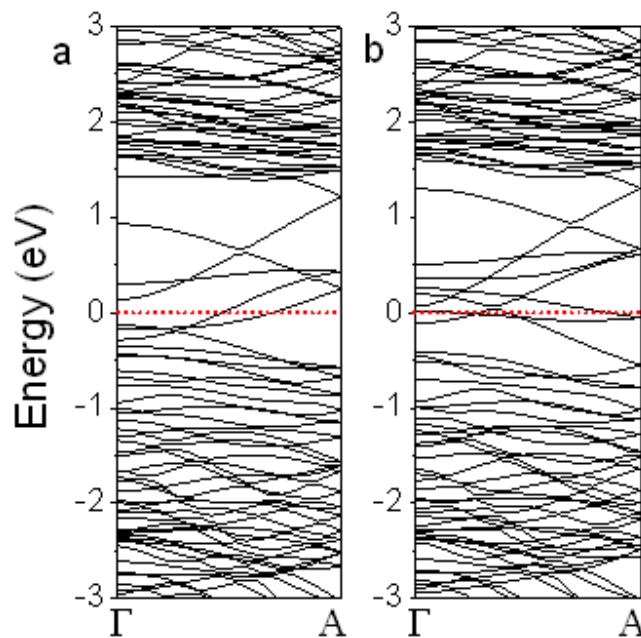
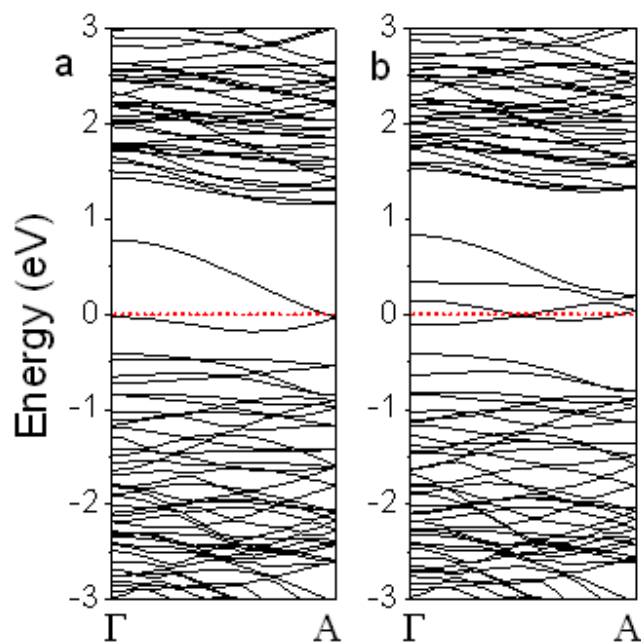


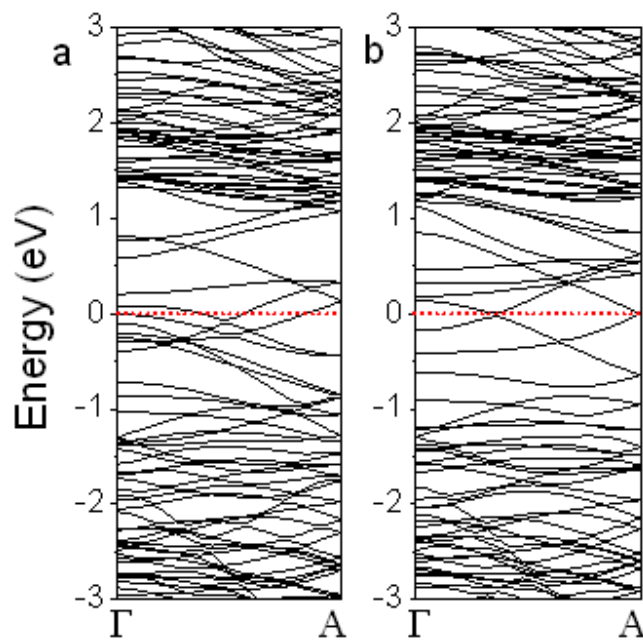
S-1, The calculated band structures of MoS₂: (a) bulk and (b) monolayer.



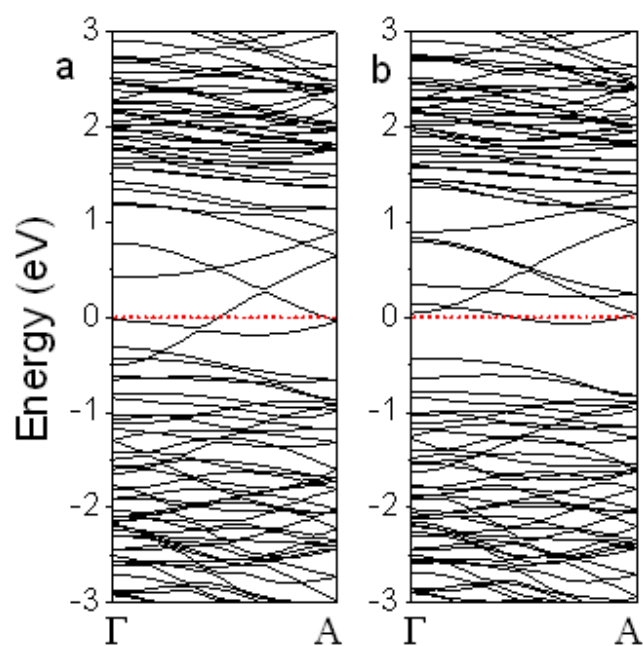
S-2, The calculated band structures of zz-MoS₂-NR-u: (a) spin-up and (b) spin-down.



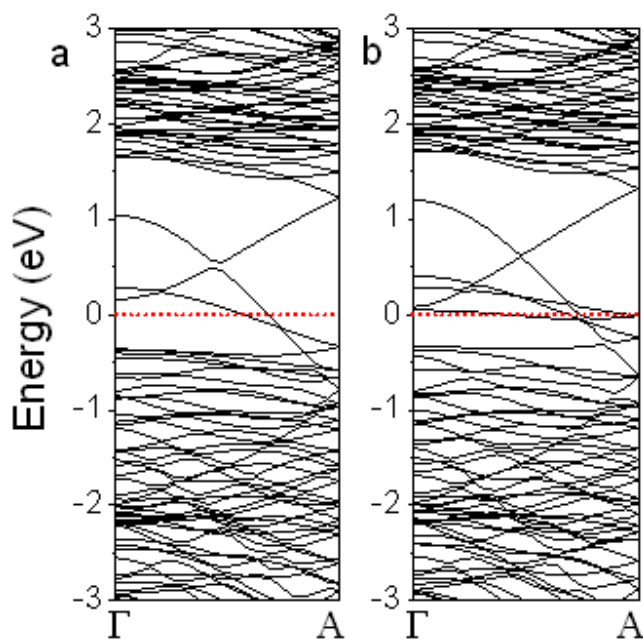
S-3, The calculated band structures of H-saturated zz-MoS₂-NR-u: (a) spin-up and (b) spin-down.



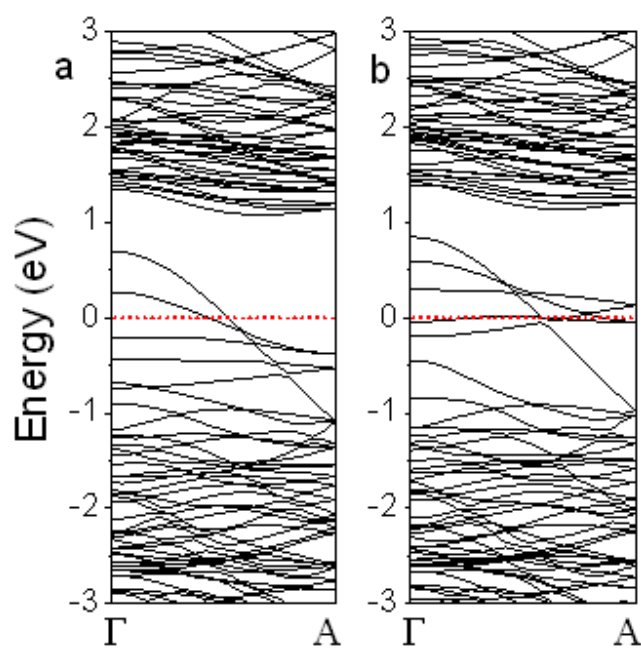
S-4, The calculated band structures of zz-MoS₂-NR-Mo-u: (a) spin-up and (b) spin-down.



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



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



S-7, The calculated band structures of H-saturated zz-MoS₂-NR-S-u: (a) spin-up and (b) spin-down.