Bidirectional heterostructures consisting of graphene and lateral MoS_2/WS_2 composites: first principles study

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Supplementary Information

Contents

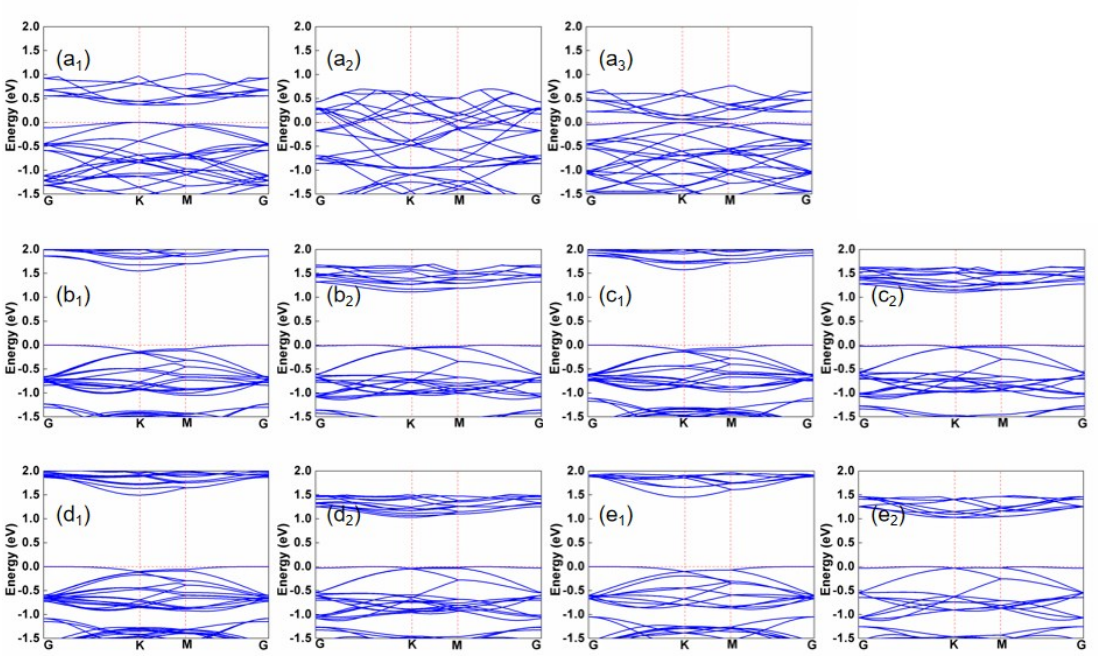

Figure S1. The band structures of WS_2 ($a_{1\text{-}2}$), $(MoS_2)_1/(WS_2)_3$ ($b_{1\text{-}2}$), $(MoS_2)_2/(WS_2)_2$ ($c_{1\text{-}2}$), $(MoS_2)_3/(WS_2)_1$ ($d_{1\text{-}2}$) and MoS_2 ($e_{1\text{-}2}$) under the electric field intensity at F= 0.5 and 1.0 V $Å^{-1}$ (1-2), and a_3 is the band structure of WS_2 at F= 0.6 V $Å^{-1}$. The horizontal red lines represent the Fermi level.

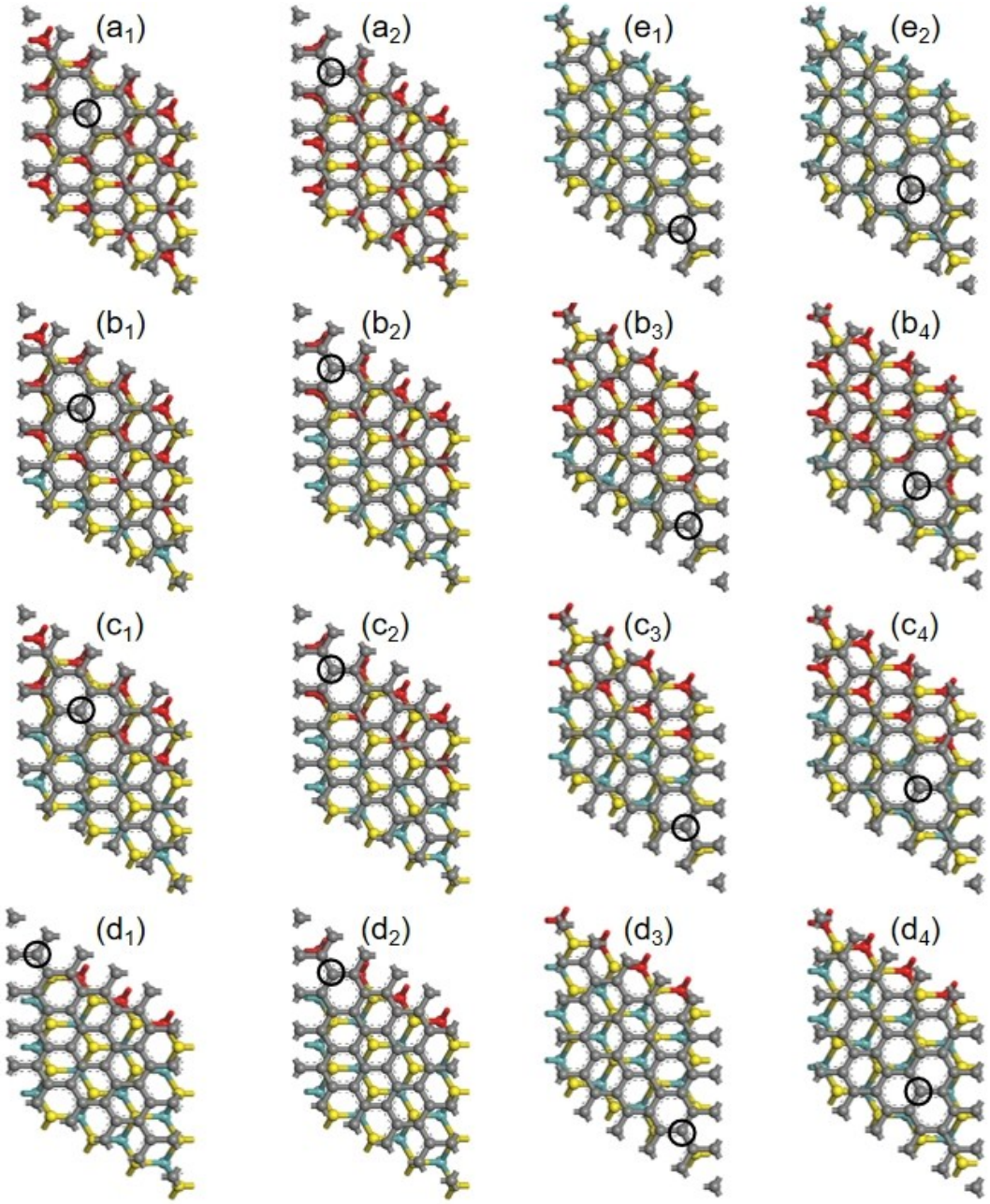

Figure S2. Top views of the configurations for G@$(MoS_2)_X/(WS_2)_{4-X}$ heterobilayer: G@WS_2 (a_{1-2}), G@$(MoS_2)_1/(WS_2)_3$ (b_{1-4}), G@$(MoS_2)_2/(WS_2)_2$ (c_{1-4}), G@$(MoS_2)_3/(WS_2)_1$ (d_{1-4}) and G@MoS_2 (e_{1-2}). The gray, yellow, green, and red balls denote C, S, Mo, W atoms, respectively.

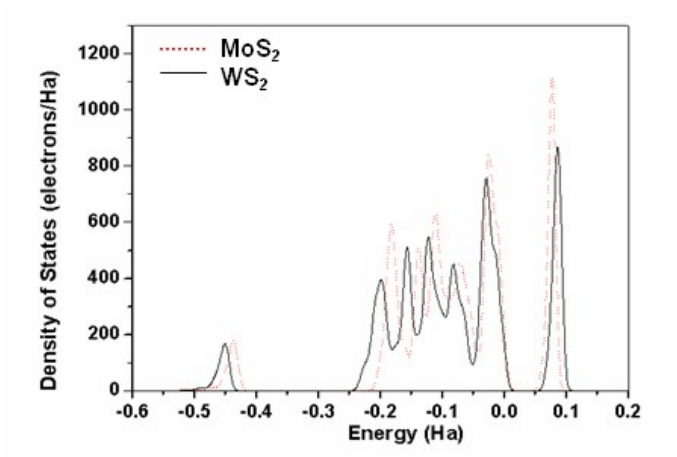

Figure S3. The PDOS of MoS_2 and WS_2.

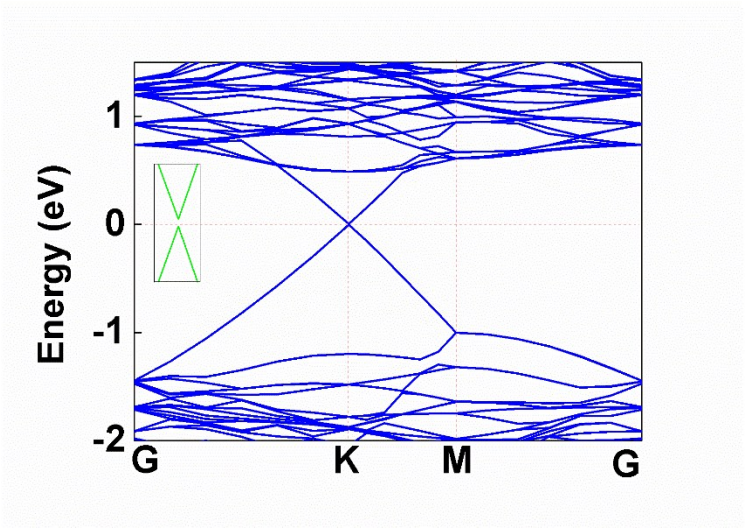

Figure S4. The band structure of G-MoS_2 at the GGA+U level.