Electronic Supplementary Material (ESI) for Nanoscale.

Half Metallic Properties of 3*d* Transition Metal Atom Intercalated Graphene@MS_2 (M=W, Mo) hybrid structures

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Supporting Information

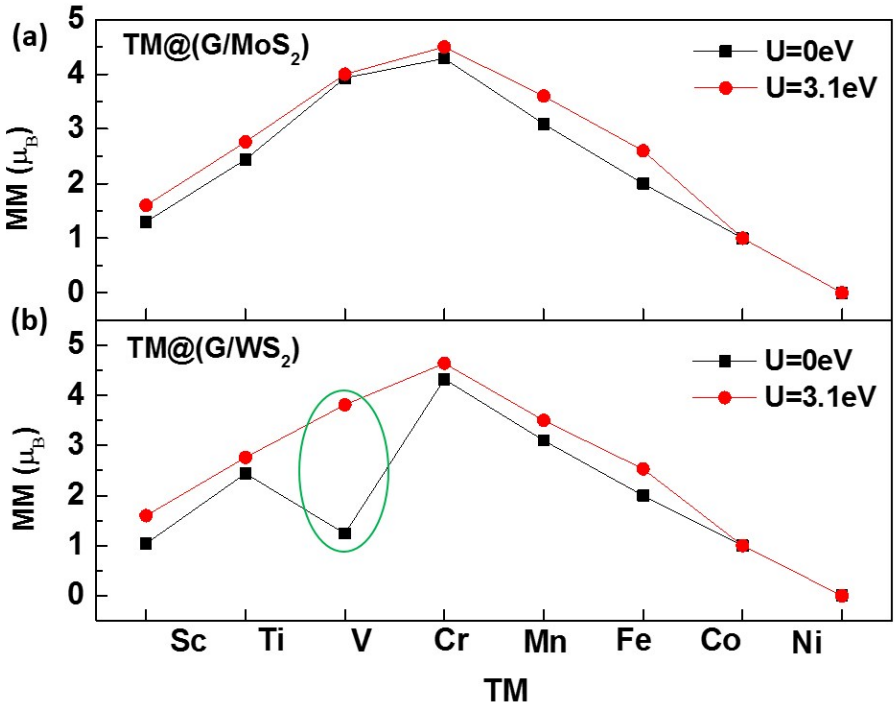

Figure S1. Compared magnetic moments of TM@(G/MoS_2) and TM@(G/WS_2) using GGA and GGA+U (Hubbard U=3.1eV) methods.

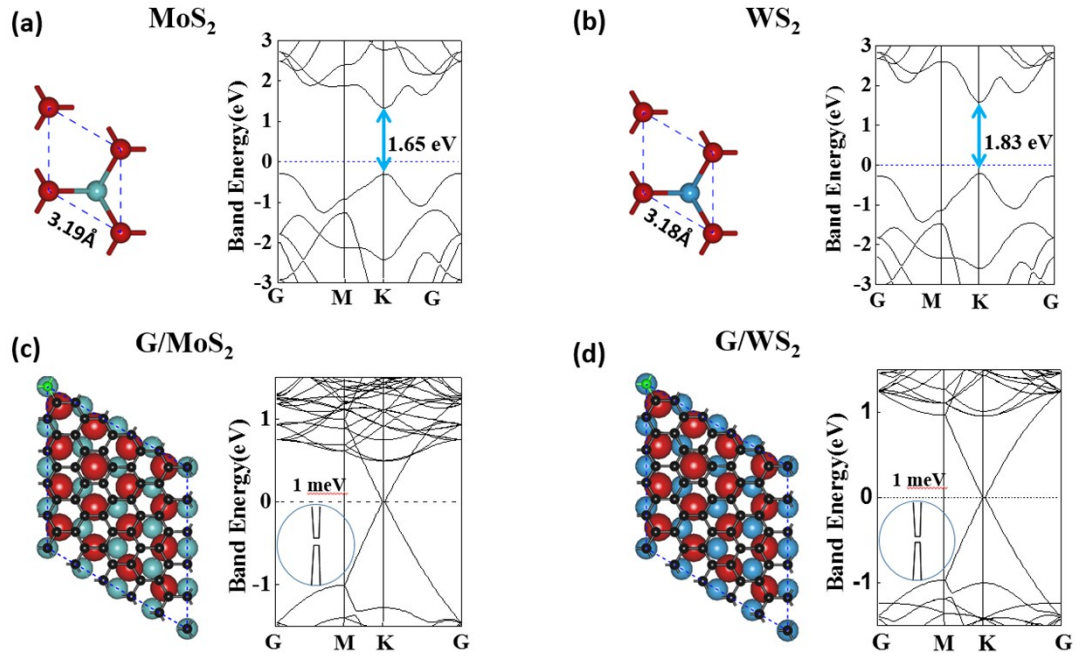

Figure S2. Geometries and bandstructures of MoS_2/WS_2 (a, b) and the G/MS_2 (M=Mo, W) heterostructures (c, d).

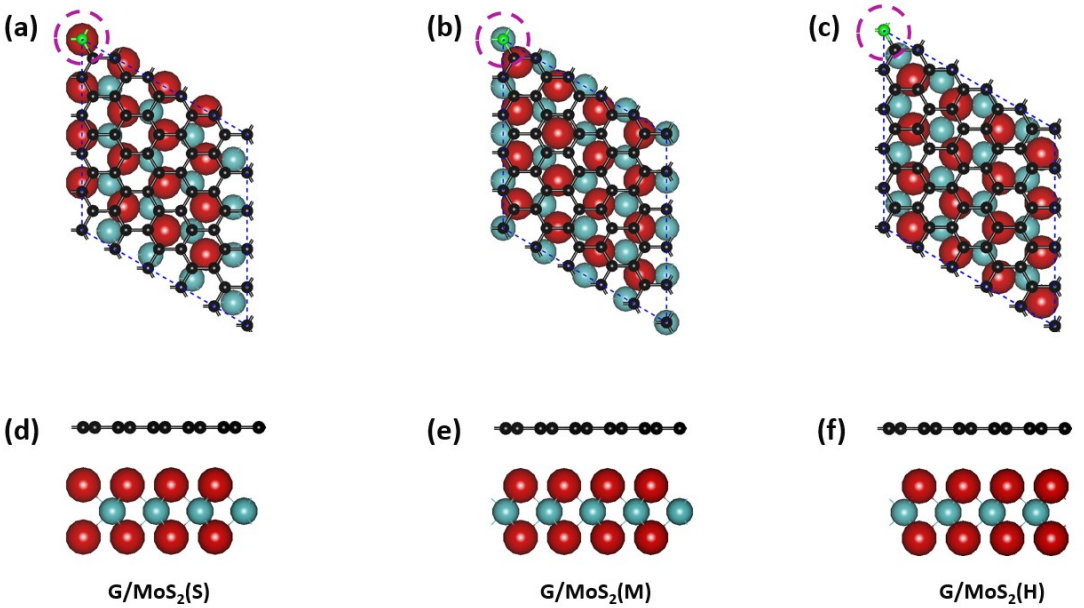

Figure S3. Top and side views of three stacking patterns of G/TMS_2s: (a, d) G/TMS_2(S) with the C atom in the upper left corner (green ball) located atop of a S atom, (b, e) G/TMS_2(TM) with the C atom in the upper left corner (green ball) located atop of a TM atom, and (c, f) G/TMS_2(H) with the C atom in the upper left corner (green ball) located on the hollow site of graphene. The red, blue, and black balls represent S, M(W, Mo), and C atoms, respectively.

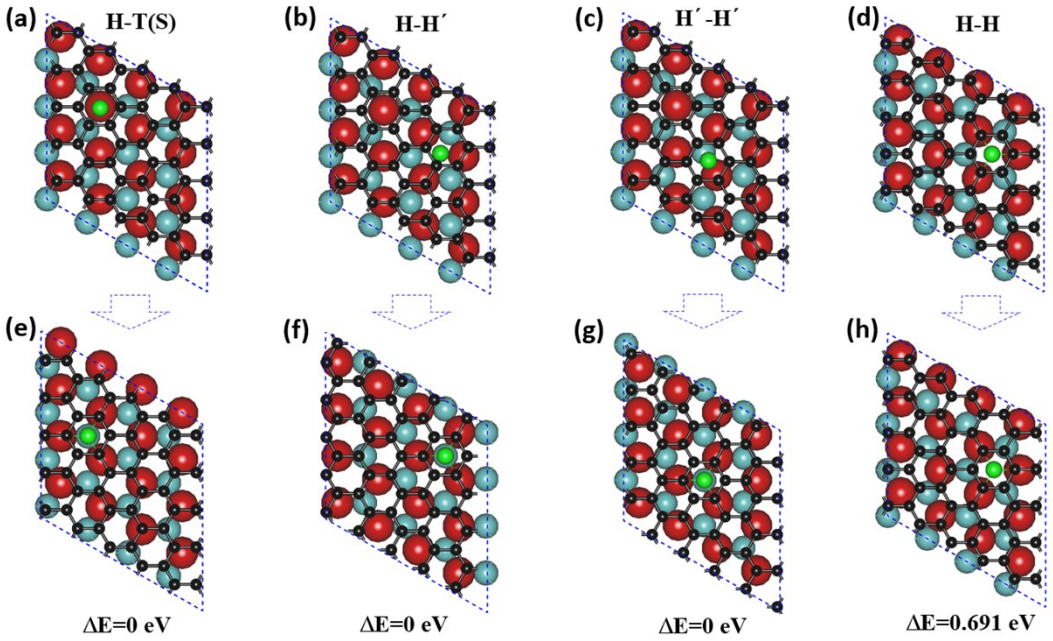

Figure S4. Initial and optimized structures of three types of Ti@(G/MoS_2), (a, e) H-T(S), (b, f) H-H´, and (c, g) H´-H´, (d, h) H-H configurations. Green, black, red and navy solid balls respect the Ti, C, S and Mo atom, respectively.

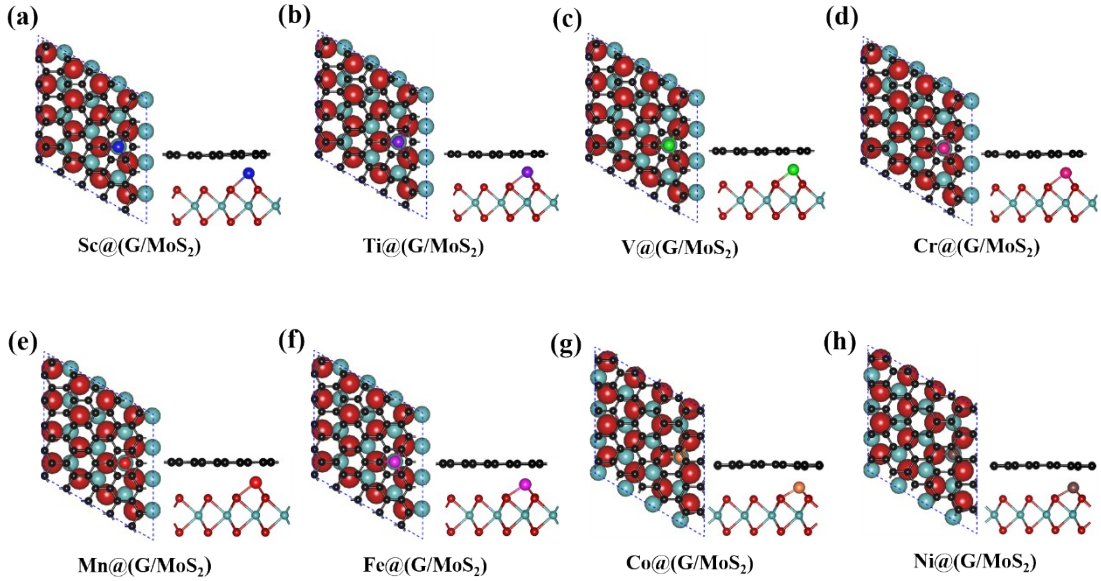

Figure S5. Optimized structures of TM@(G/MoS_2) , TM=S-Ni.

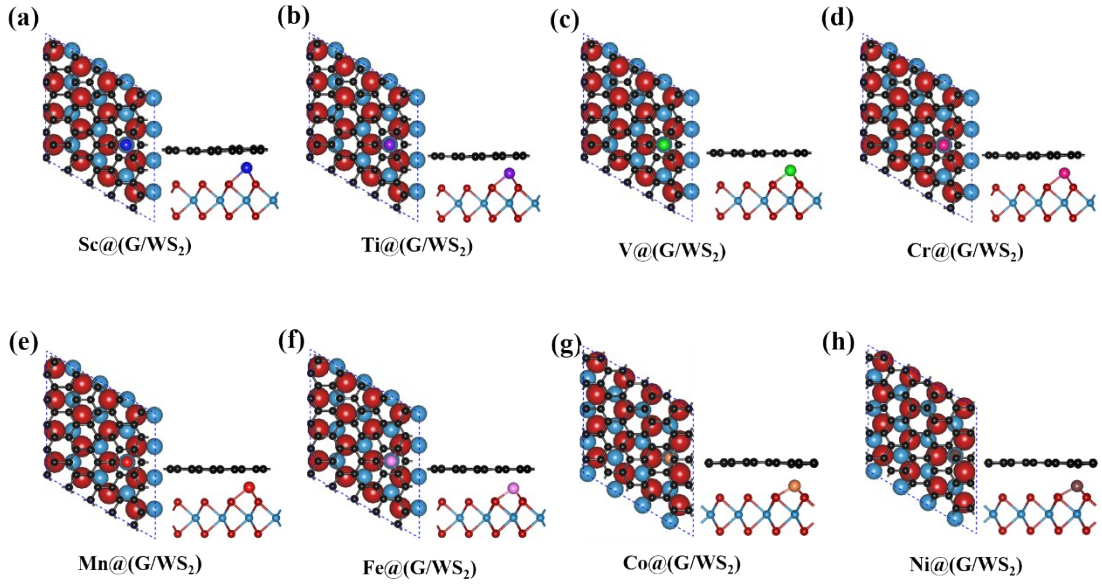

Figure S6. Optimized structures of TM@(G/WS_2) , TM=S-Ni.

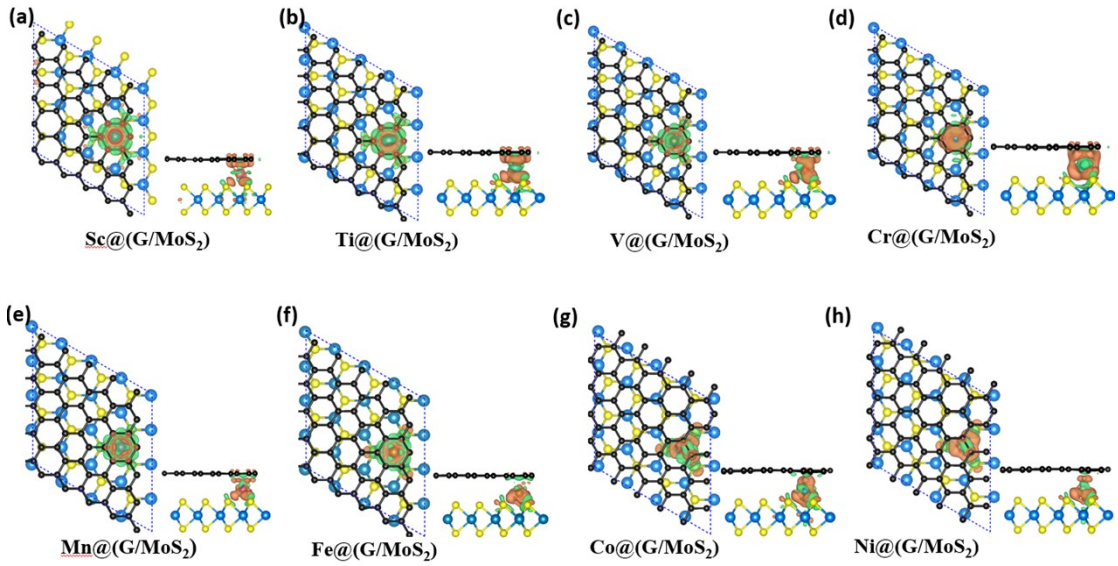

Figure S7. Charge density differences of TM@(G/MoS_2), TM=Sc-Ni.

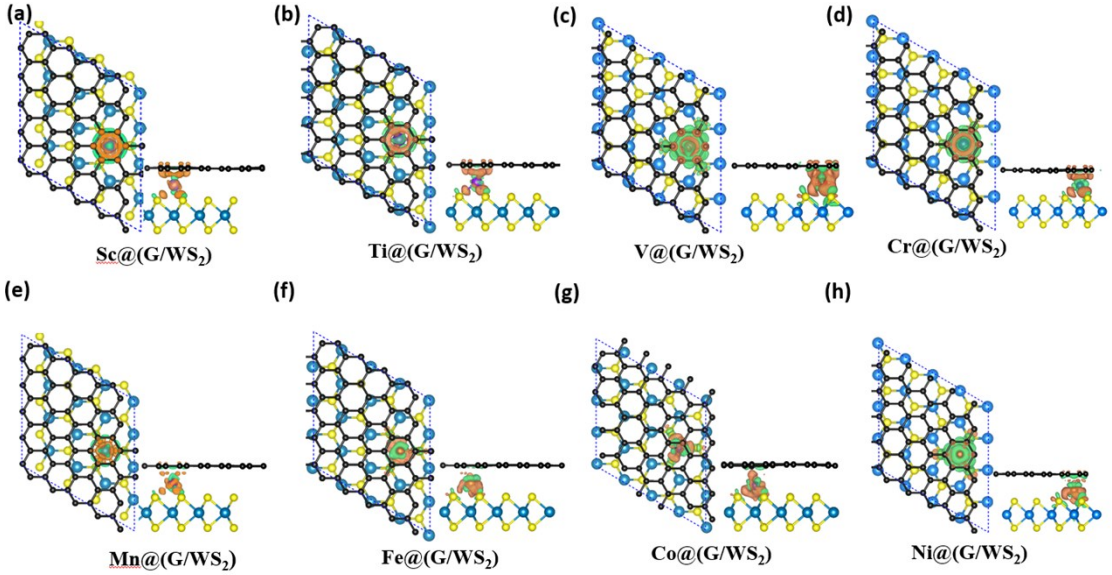

Figure S8. Charge density differences of TM@(G/WS_2), TM=Sc-Ni.

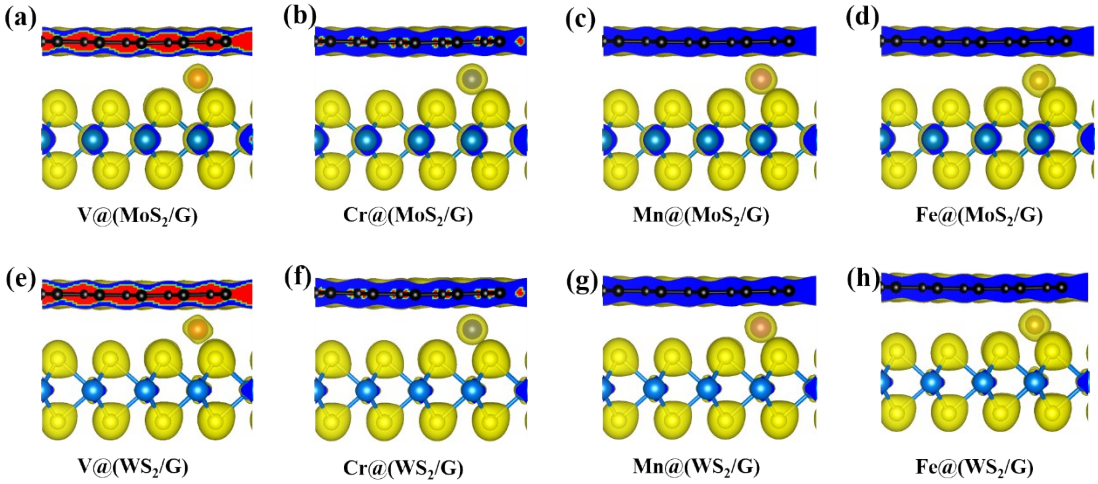

Figure S9. Charge density plots of TM@(G/MoS_2) and TM@(G/WS_2) , TM=V, Cr, Mn, Fe.

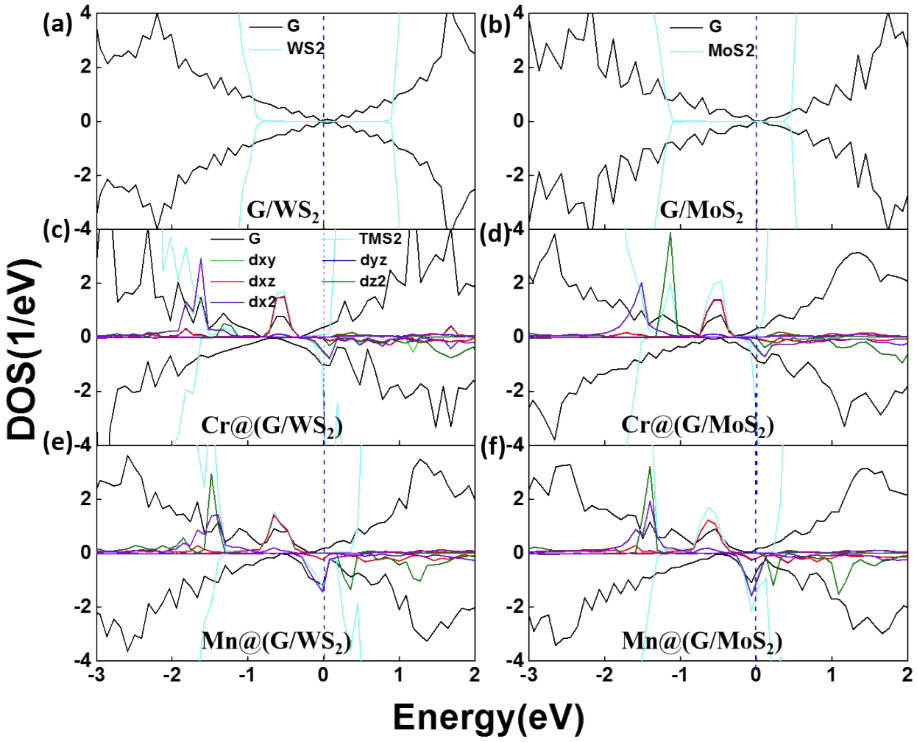

Figure S10. (a-h)The density of states (DOS) of G/WS_2, G/MoS_2 and $TM@(G/WS_2)$, $TM@(G/MoS_2)$,TM=Cr,Mn.

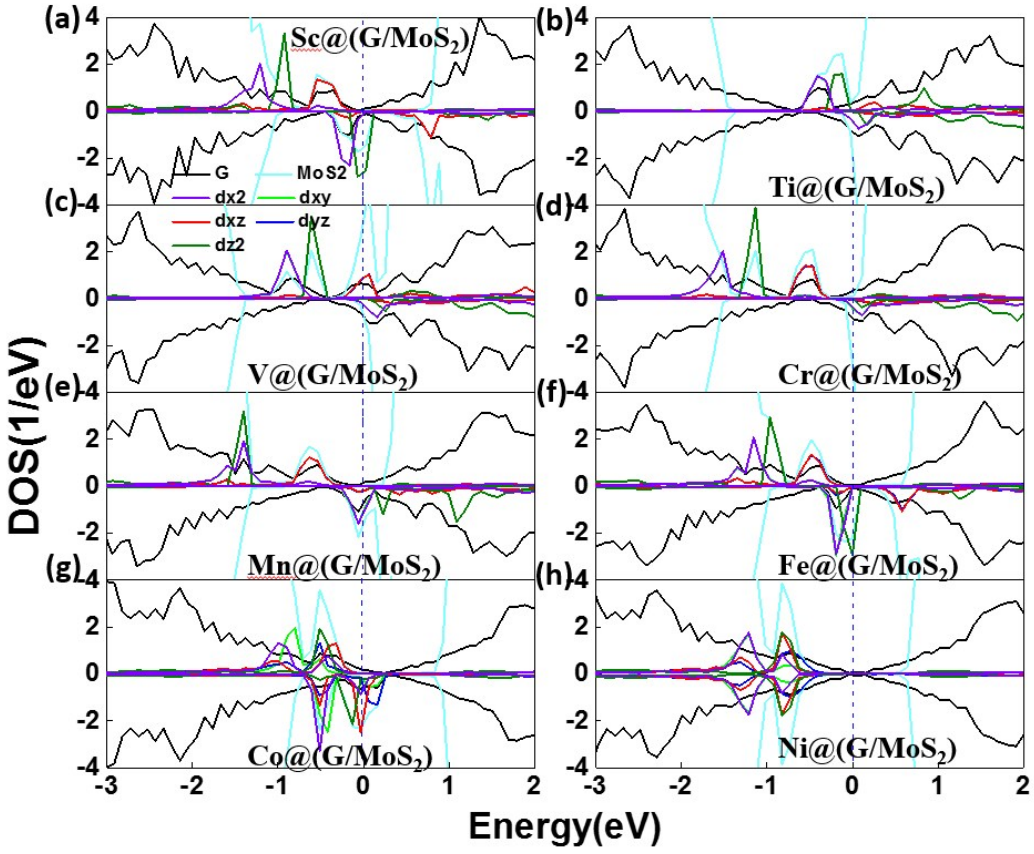

Figure S11. (a-h)The density of states (DOS) $TM@(G/WS_2)$,TM=Sc-Ni.

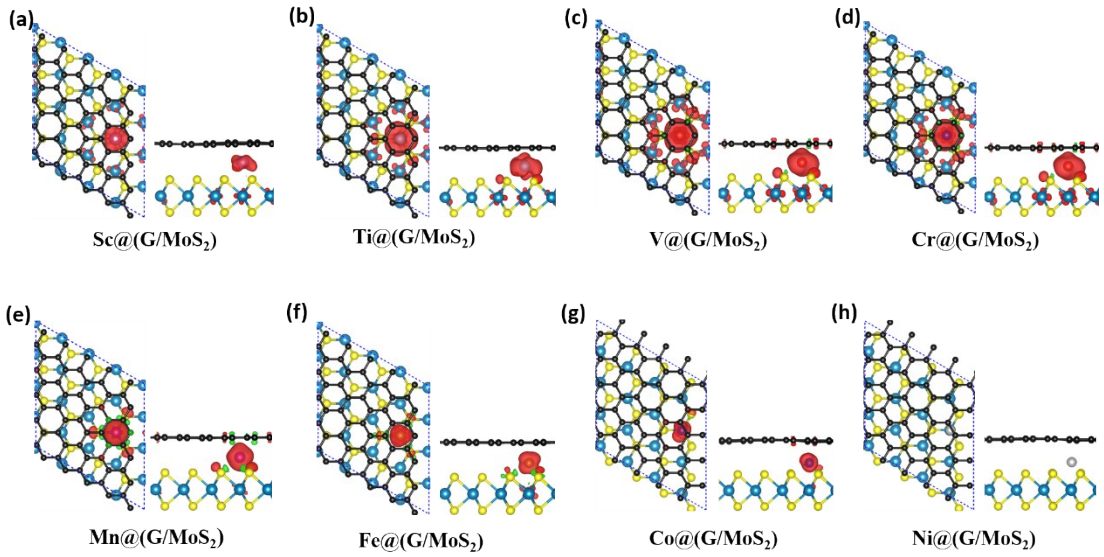

Figure S12. (a-h)The spin density plots of TM@(G/MoS_2),TM=Sc-Ni.

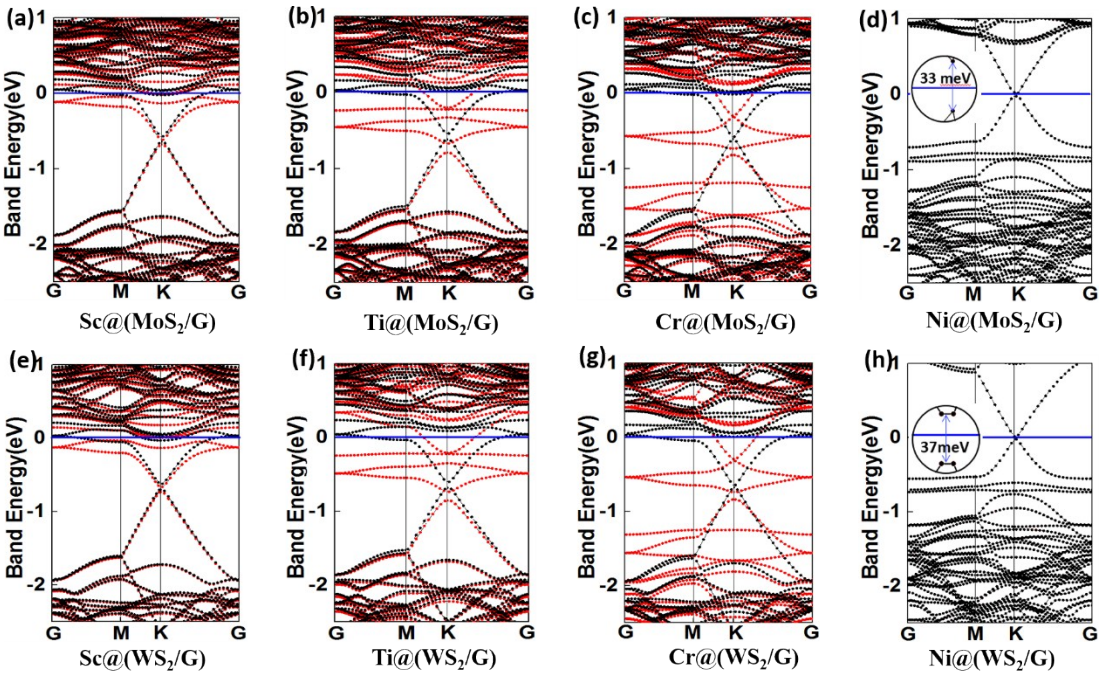

Figure S13. The band structures of TM@(G/MoS_2) (a-d) and TM@(G/WS_2) (e-h),TM=Sc, Ti, Cr, Ni.

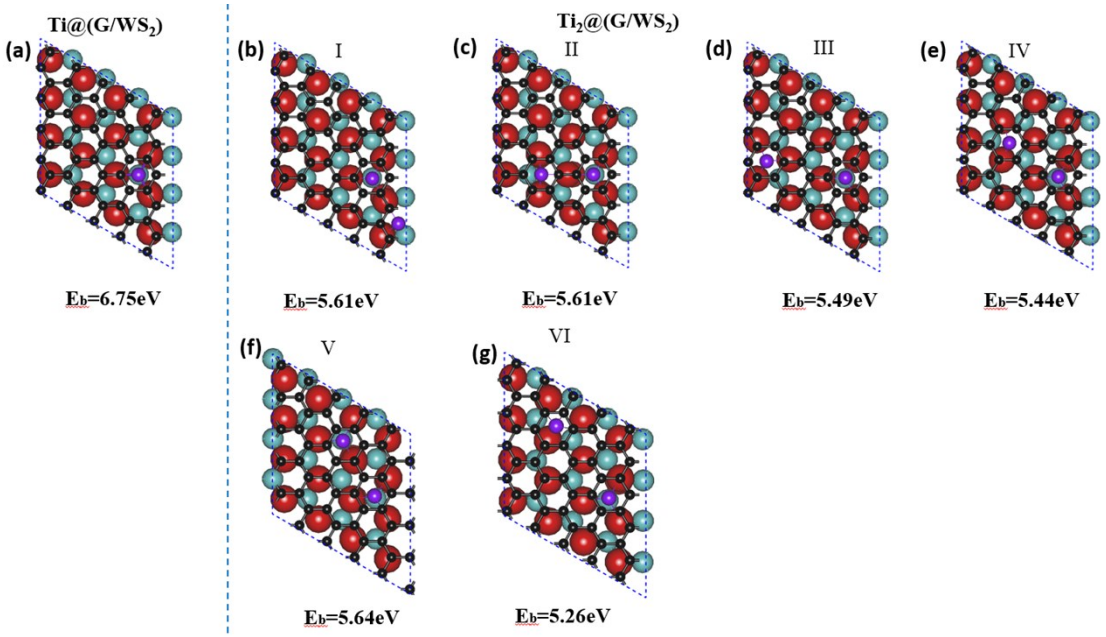

Figure S14. The structures and binding energies of (a) Ti@(G/MS_2) and (b-g) six Ti_2@(G/MS_2) isomers.

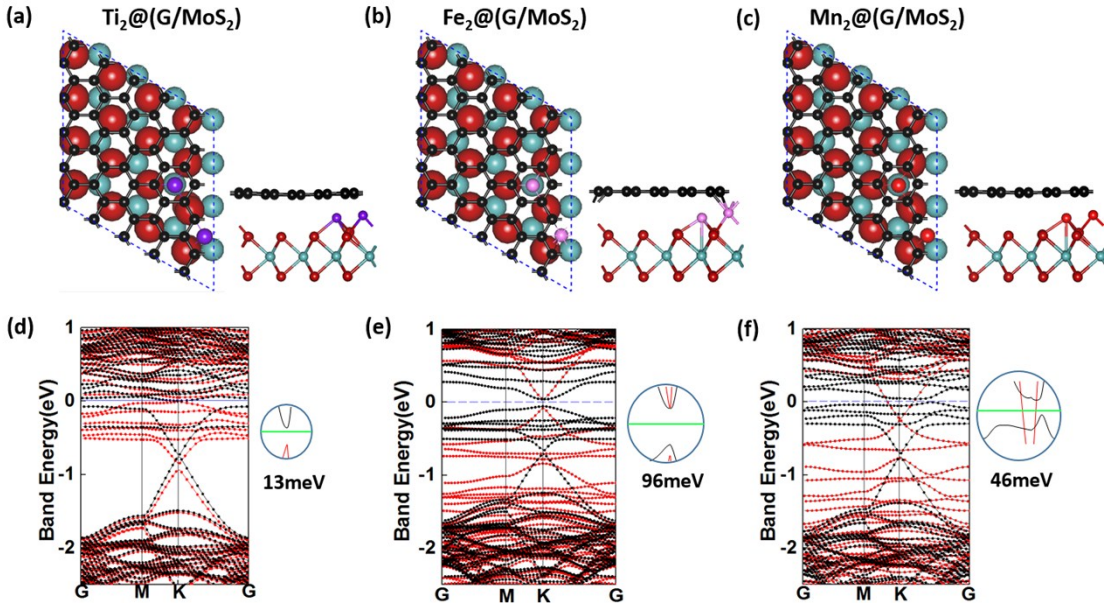

Figure S15. The structures (a-c) and band structures (d-f) of Ti_2@(G/MoS_2), Fe_2@(G/MoS_2) Mn_2@(G/MoS_2).