Half Metallic Properties of 3d Transition Metal Atom Intercalated Graphene@MS\textsubscript{2} (M=W, Mo) hybrid structures

Xiuyun Zhang*, Zujian Bao, Xiaoshan Ye, Wenxian Xu, Qiang Wang, Yongjun Liu*
College of Physics Science and Technology, Yangzhou University, Yangzhou, 225002

Supporting Information

Figure S1. Compared magnetic moments of TM@(G/MoS\textsubscript{2}) and TM@(G/WS\textsubscript{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$_2$: (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=S-Ni.
Figure S8. Charge density differences of $\text{TM}@\text{(G/WS}_2\text{)}$, TM=Sc-Ni.

Figure S9. Charge density plots of $\text{TM}@\text{(G/MoS}_2\text{)}$ and $\text{TM}@\text{(G/WS}_2\text{)}$, 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}) and Mn_{2}@((G/MoS)_{2}).