

Supporting Information

Tunable Electronic and Magnetic Properties of 3d Transition Metal Atom-Intercalated Transition Metal Dichalcogenides: A Density Functional Theory Study

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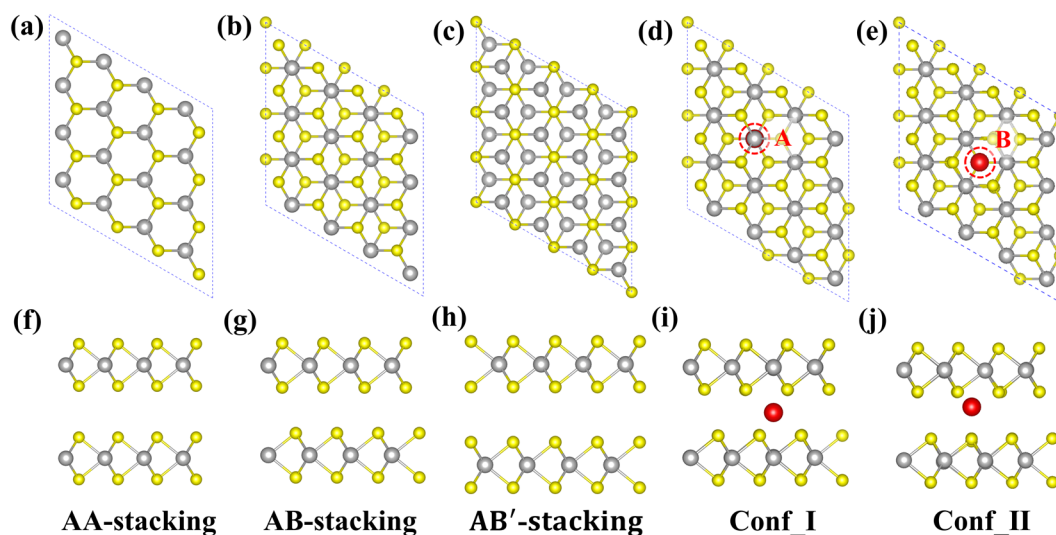


Figure S1. Top and side views of (a,f) AA-, (b,g) AB-, and (c,h) AB'-stacking of bilayer VS₂. Top and side views of TM@BL_VS₂ with TM intercalating at the (d,i) A site and (e,j) B site.

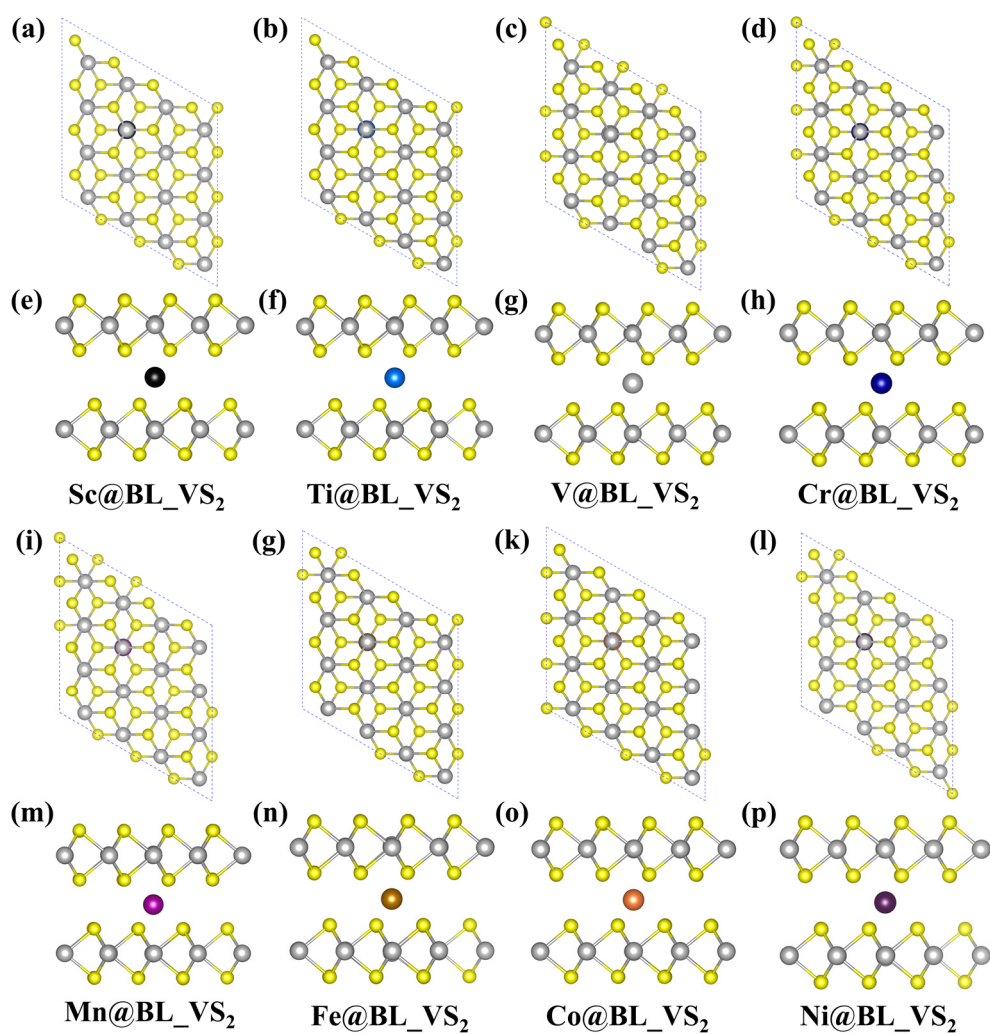


Figure S2. (a–d,i–l) Top views and (e–h,m–p) side views of the optimized structures for TM@BL_VS₂s (TM= Sc–Ni).

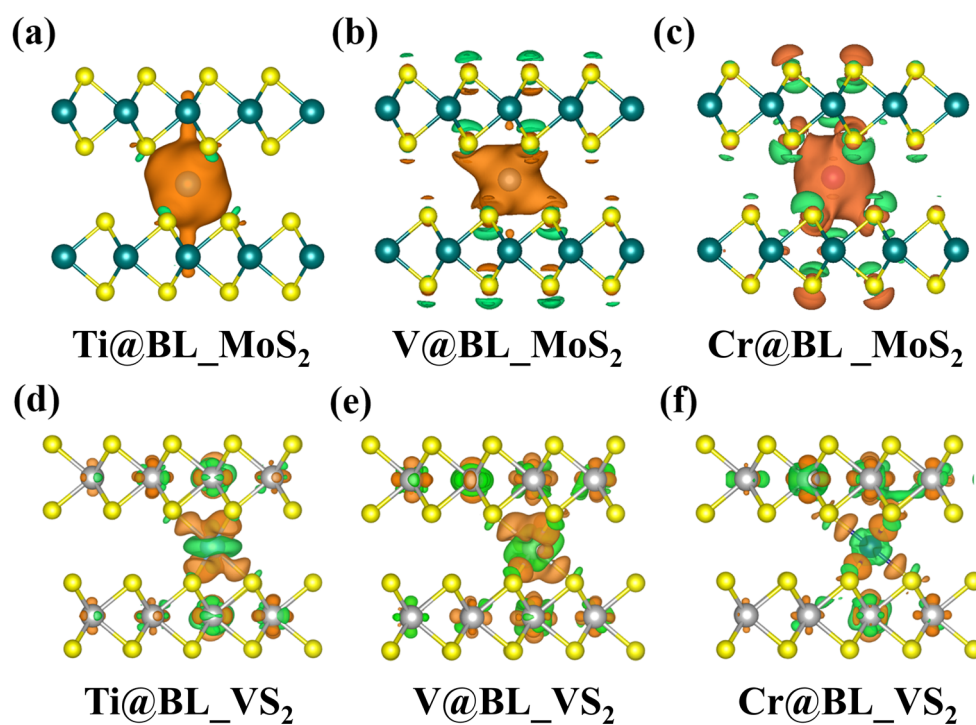


Figure S3. (a–c) The CDDs plots of TM@BL_MoS_2 (TM = Ti, V, Cr). (d–f) The CDDs plots of TM@BL_VS_2 (TM = Ti, V, Cr).

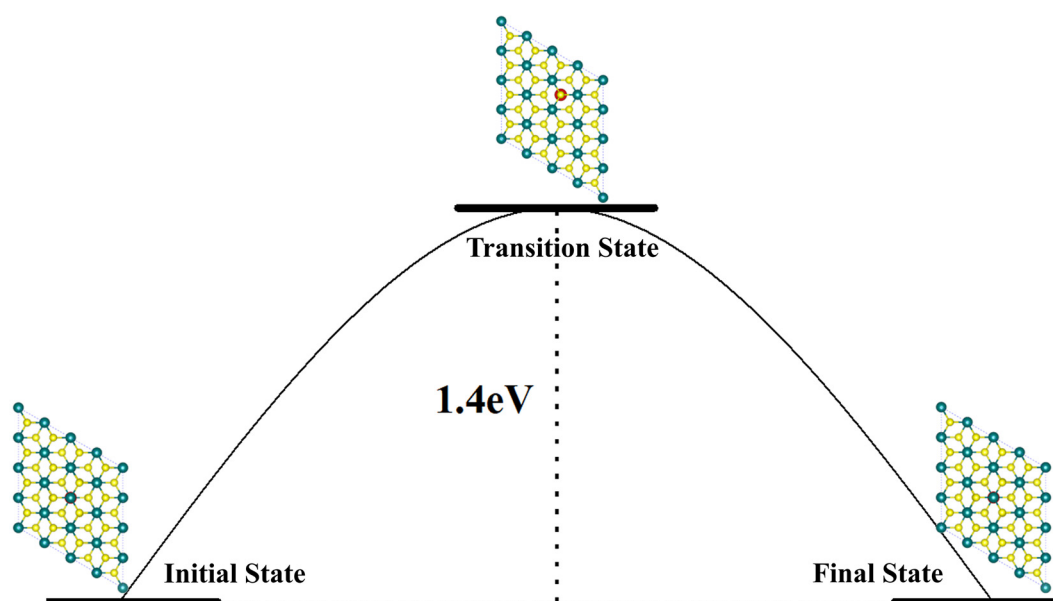


Figure S4. Energy barrier for Ti@BL_MoS_2 diffusion from position A to position B.

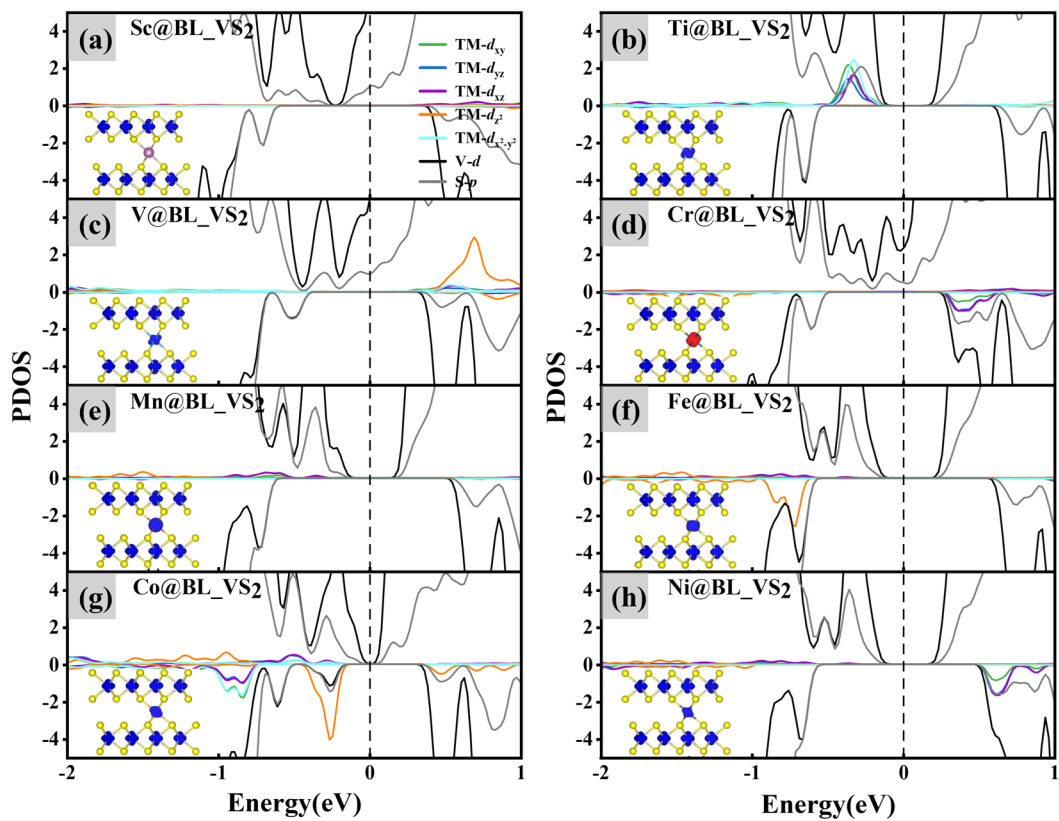


Figure S5. (a–h) Partial density of states (PDOS) and spin density plots for TM@BL_VS₂ (TM = Sc–Ni). Inside the PDOS graph is its corresponding spin density graph; blue represents positive spin, and red represents negative spin.

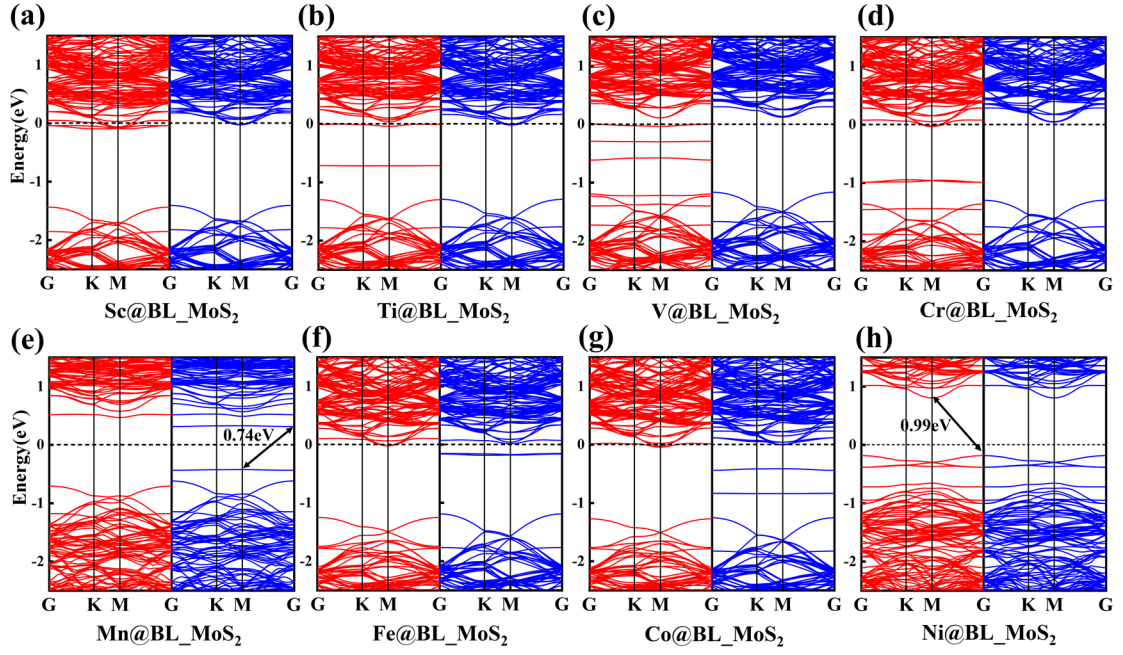


Figure S6. (a–h) Band structures of TM@BL_MoS₂ (TM = Sc–Ni). Red and blue lines represent up and down spin, respectively.

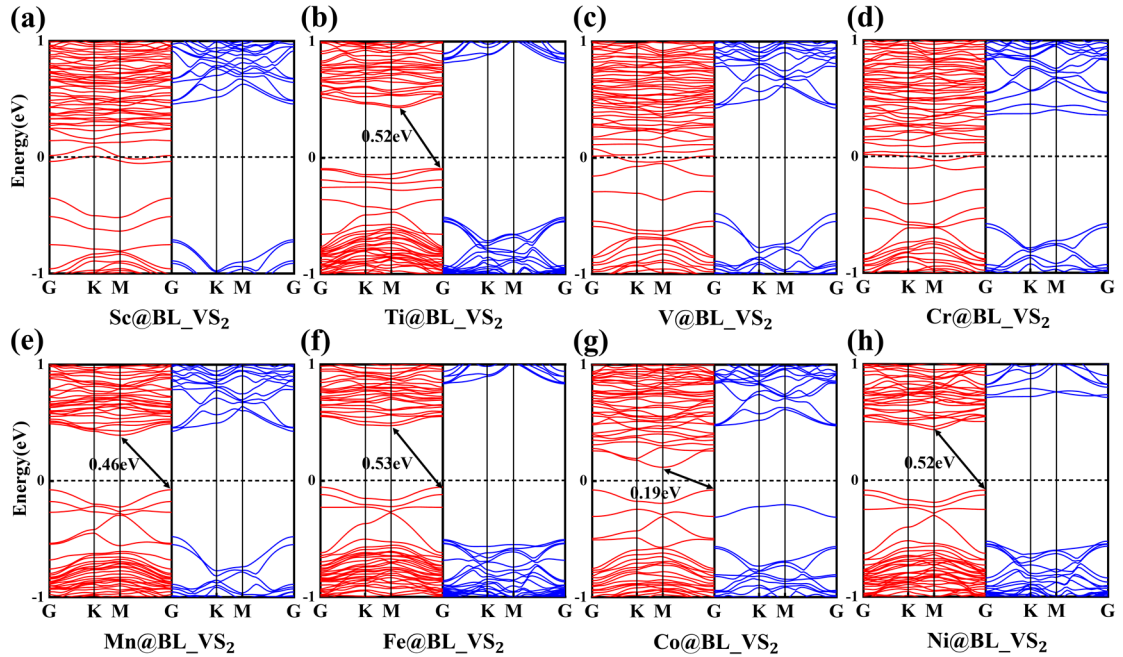


Figure S7. (a–h) Band structures of TM@BL_VS₂ (TM = Sc–Ni). Red and blue lines represent up and down spin, respectively.

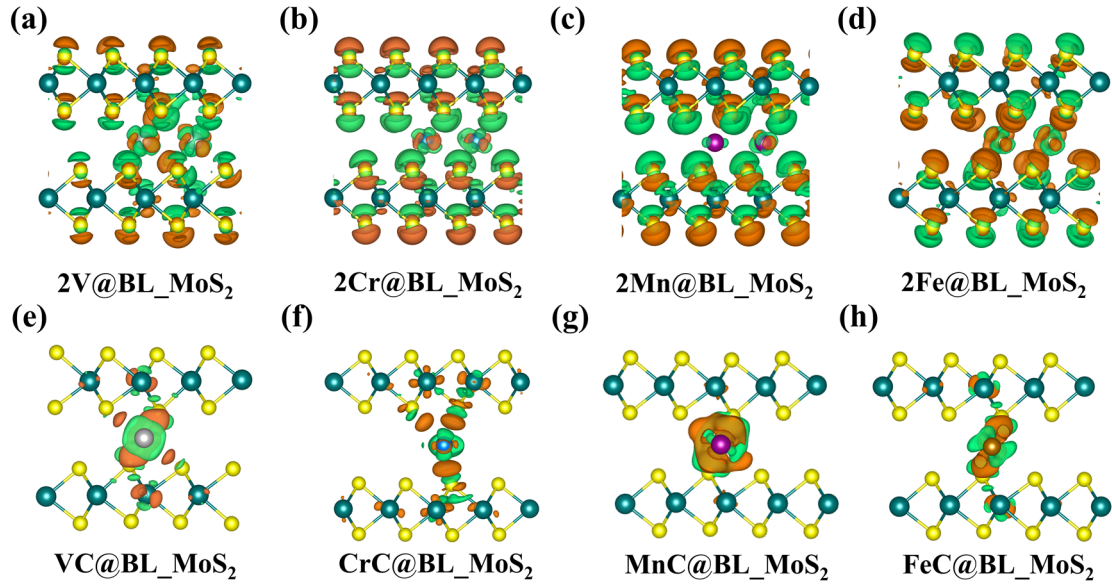


Figure S8. (a–d) The CDDs plots of $2TM@BL_MoS_2$ (TM = V, Cr, Mn, Fe). (e–h) The CDDs plots of $TMC@BL_MoS_2$ (TM = V, Cr, Mn, Fe).

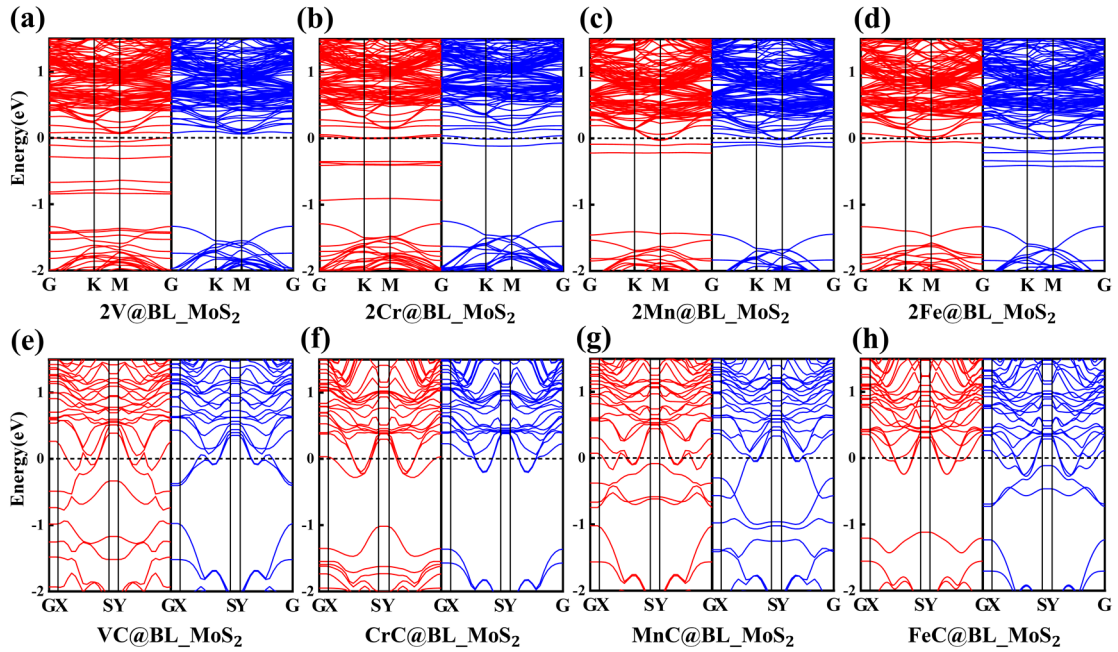


Figure S9. (a–d) Band structures of $2TM@BL_MoS_2$ (TM = V, Cr, Mn, Fe). (e–h) Band structures of $TMC@BL_MoS_2$ (TM = V, Cr, Mn, Fe). Red and blue lines represent up and down spin, respectively.