Electronic Supplementary Material (ESI) for RSC Advances.

Sizable Bandgaps of graphene in 3*d* Transition Metal Intercalated Defected Graphene/WSe_2 Heterostructures

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Supporting Information

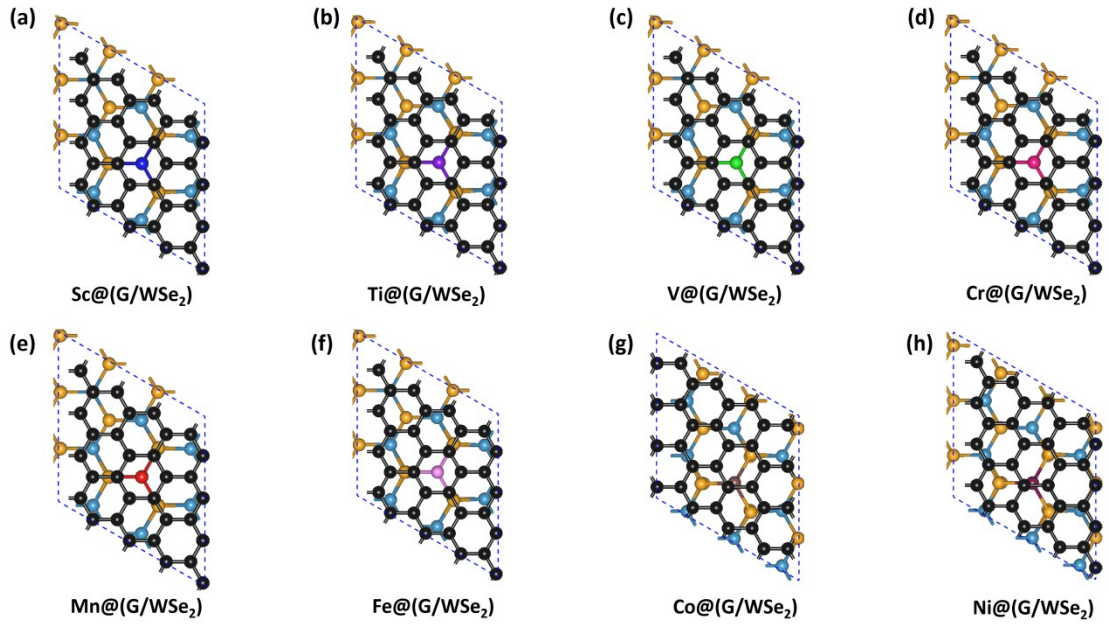

Figure S1. Optimized structures of TM@(G/WSe_2)s, TM=Sc-Ni. Black, blue and yellow balls represent the C, W and Se atoms, respectively.

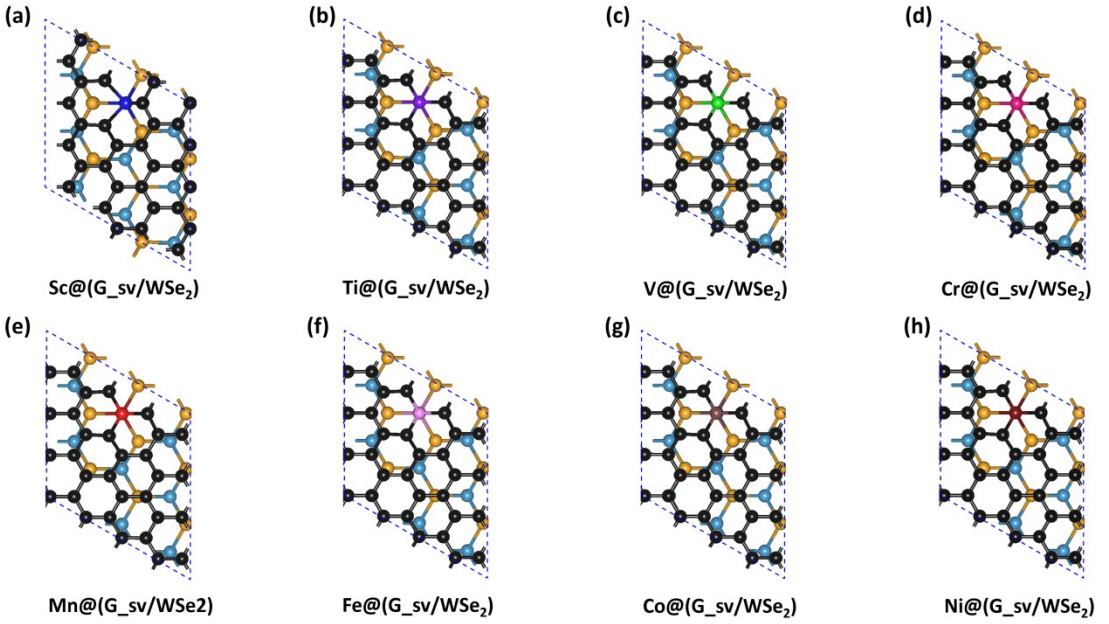

Figure S2. Optimized structures of TM@(G_sv/WSe_2)s, TM=Sc-Ni. Black, blue and yellow balls represent the C, W and Se atoms, respectively.

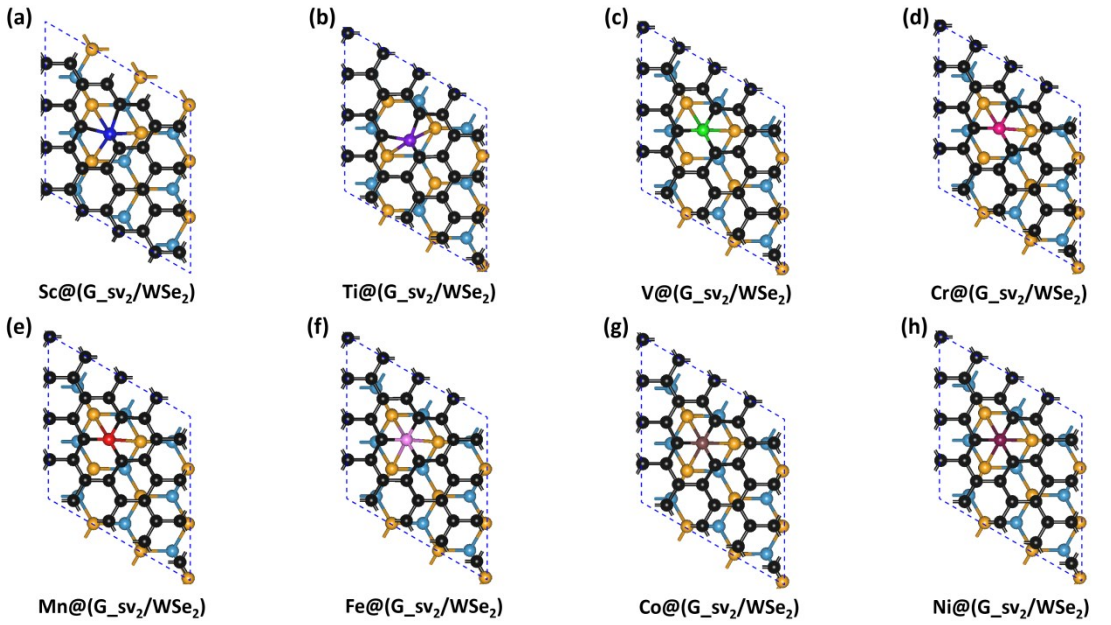

Figure S3. Optimized structures of TM@(G_sv_2/WSe_2)s, TM=Sc-Ni. Black, blue and yellow balls represent the C, W and Se atoms, respectively.

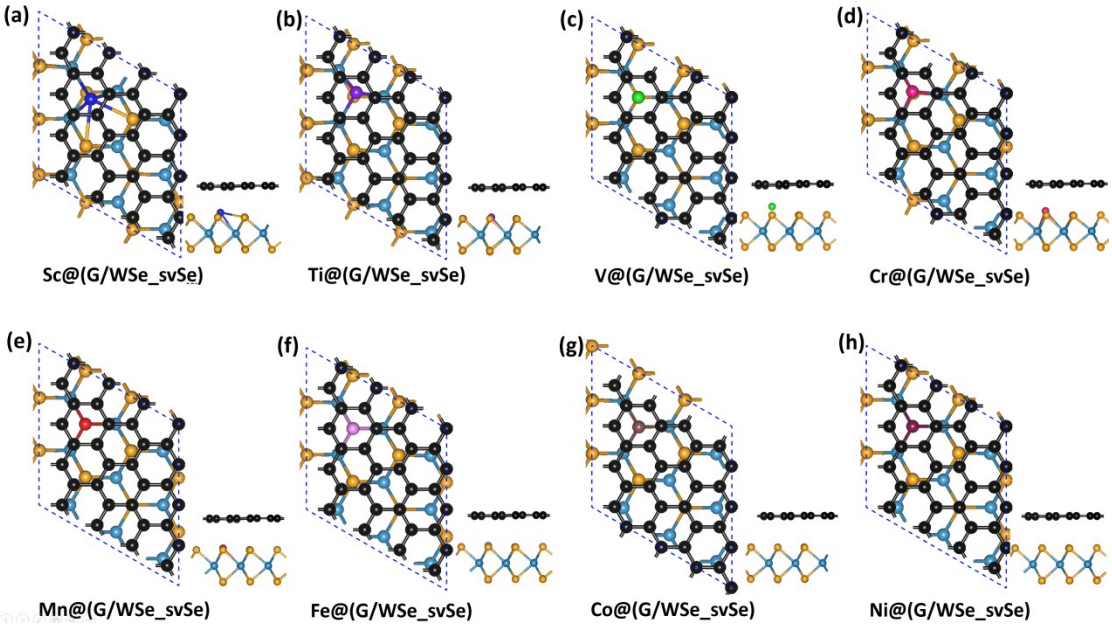

Figure S4. Optimized structures of TM@(G/WSe_svSe)s, TM=Sc-Ni. Black, blue and yellow balls represent the C, W and Se atoms, respectively.

Table S1. The distance of TM atoms to the graphene layer (D_{TM-G}, Å) and WSe_2 layer ($D_{TM-WSe2}$, Å), the total magnetic moments (MM, μ_B) the band gap (Δ, eV) of half metals and semiconductors, the metallic properties of the TM@(G/WSe_2)s systems.

Sys	D_{TM-G}(Å)	$D_{TM-WSe2}$(Å)	MM(μ_B)	Δ(eV)(metallic)
Sc@(G/WSe_2)	1.81	1.68	1.80	0(metal)
Ti@(G/WSe_2)	1.8	1.53	2.46	0(metal)
V@(G/WSe_2)	1.74	1.49	3.81	0.23(HM)
Cr@(G/WSe_2)	1.82	1.53	4.30	0(metal)
Mn@(G/WSe_2)	1.74	1.55	3.05	0.13(HM)
Fe@(G/WSe_2)	1.79	1.44	2.02	0.05(HM)
Co@(G/WSe_2)	2.17	1.14	1.02	0.06(HM)
Ni@(G/WSe_2)	2.25	1.11	0	0.06(SC)

Table S2. The distance of TM atoms to the graphene layer (D_{TM-G}, Å) and WSe_2 layer ($D_{TM-WSe2}$, Å), the total magnetic moments (MM, μ_B) and the band gap (Δ, eV) of half metallic and semiconducting TM@(G_sv/WSe_2)s and TM@(G_sv_2/WSe_2)s. Numbers of "1" and "2" represent the related information for TM@(G_sv/WSe_2)s and TM@(G_sv_2/WSe_2)s, respectively.

Sys	$D_{TM-G1,2}$ (Å)	$B_{TM-Se1,2}$(Å)	$MM_{1,2}$(μ_B)	$\Delta_{1,2}$(eV）
Sc@(G_sv/WSe_2)	1.08/1.04	2.80-2.81/2.79-2.89	0.72/0.32	0.39(HM)/0(metal)
Ti@(G_sv/WSe_2)	1.22/1.00	2.74-2.75/2.70-2.72	0/0	0.10(HM)/0.09(HM)
V@(G_sv/WSe_2)	1.16/1.11	2.67-2.68/2.73-2.77	1.0/1.0	0.13(HM)/0.29(SC)
Cr@(G_sv/WSe_2)	1.11/1.08	2.66-2.66/2.66-2.80	2.0/2.0	0.27(HM)/0.22(HM)

Mn@(G_{sv}/WSe_2)	1.08/1.05	2.70-2.71/2.68-2.82	2.93/2.98	0(metal)/0(metal)
Fe@(G_{sv}/WSe_2)	1.00/0.94	2.63-2.64/2.62-2.78	0/0	0.51(SC)/0.39(SC)
Co@(G_{sv}/WSe_2)	1.01/0.98	2.65-2.69/ 2.68-2.73	0.96/0.88	0.58(HM)/0.52(HM)
Ni@(G_{sv}/WSe_2)	1.05/1.04	2.69-2.69/2.68-2.72	0/0	0.29(SC)/0.30(SC)

Table S3. The distance of graphene layer and WSe_2 layer (D_{layer}, Å), the total magnetic moments (MM,μ_B) and the metallic properties of the TM@(G/WSe_svSe)s.

Sys	D_{layer}(Å)	MM(μ_B)	metallic
Sc@(G/WSe_svSe)	3.32	0.69	metal
Ti@(G/WSe_svSe)	3.3	0	metal
V@(G/WSe_svSe)	3.29	4.82	metal
Cr@(G/WSe_svSe)	3.33	0.19	metal
Mn@(G/WSe_svSe)	3.35	3.02	metal
Fe@(G/WSe_svSe)	3.32	2.30	metal
Co@(G/WSe_svSe)	3.35	1.03	metal
Ni@(G/WSe_svSe)	3.35	0	metal

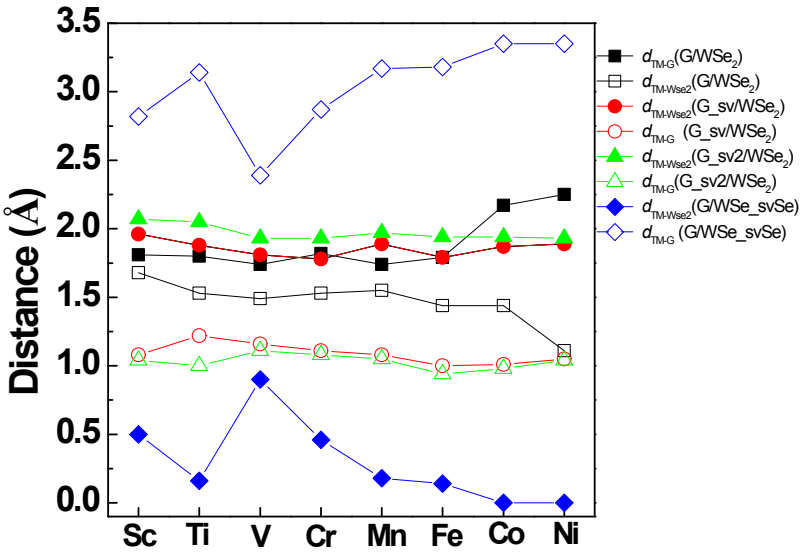

Figure S5. The distances of TM atoms to the graphene layer and WSe_2 layer in TM@(G /WSe_2)s, TM@(G_sv/WSe_2)s, TM@(G_sv_2/WSe_2)s and TM@(G/WSe_svSe)s, respectively.

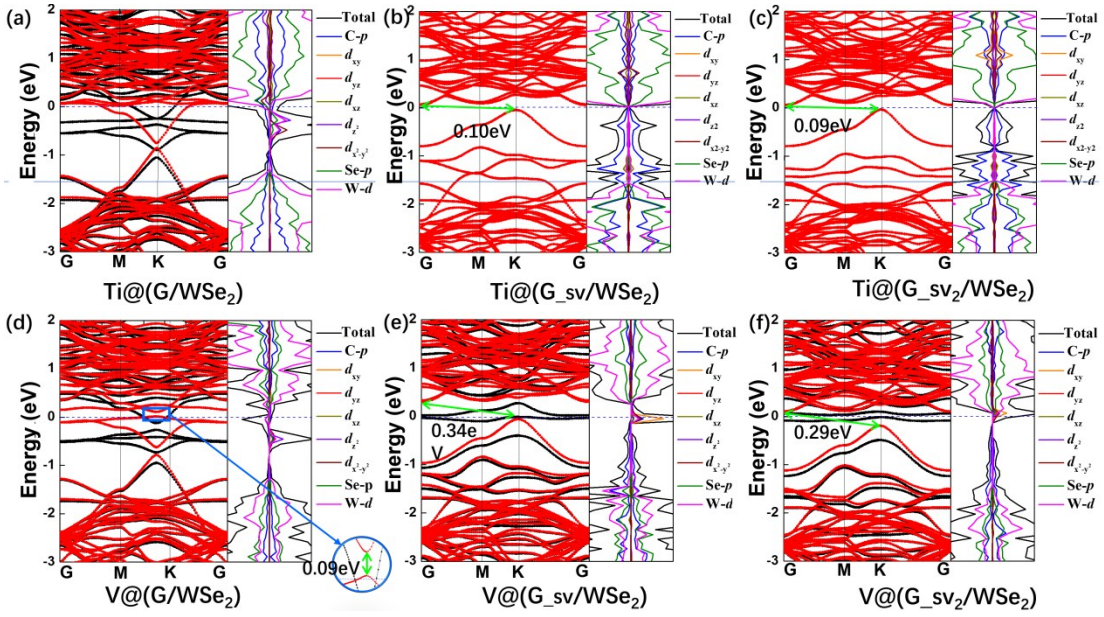

Figure.S6. (a-f) Plots of band structures and density of states (DOS) of TM@(G/WSe_2)s, TM@(G_sv/WSe_2)s and TM@(G_sv_2/WSe_2)s, TM=Ti, V, respectively.

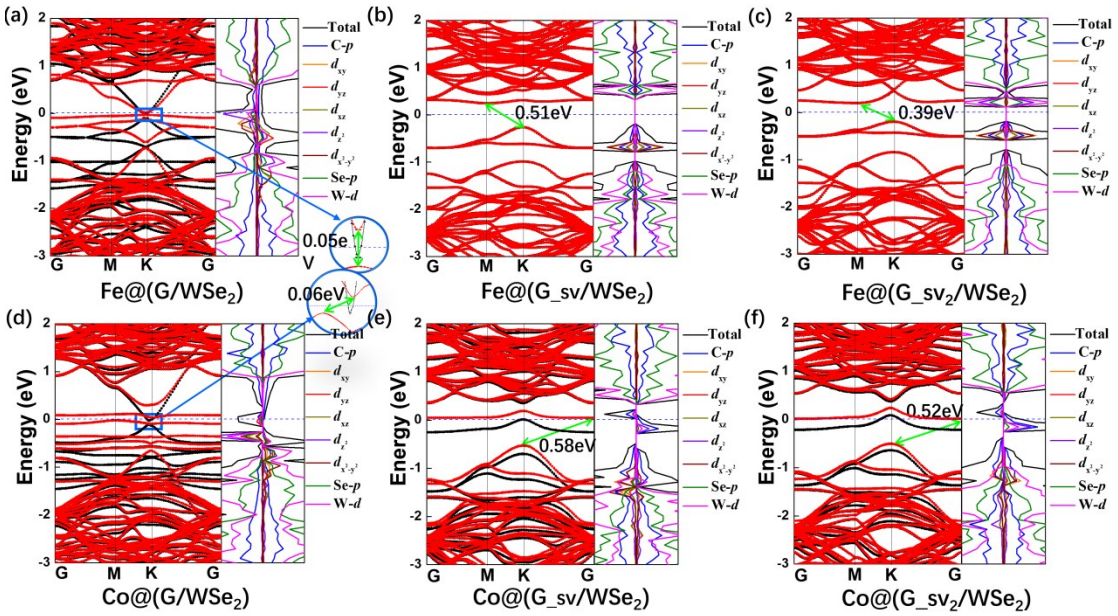

Figure S7. (a-f) Plots of band structures and density of states (DOS) of TM@(G/WSe_2)s, TM@(G_sv/WSe_2)s and TM@(G_sv_2/WSe_2)s, TM=Fe, Co, respectively.

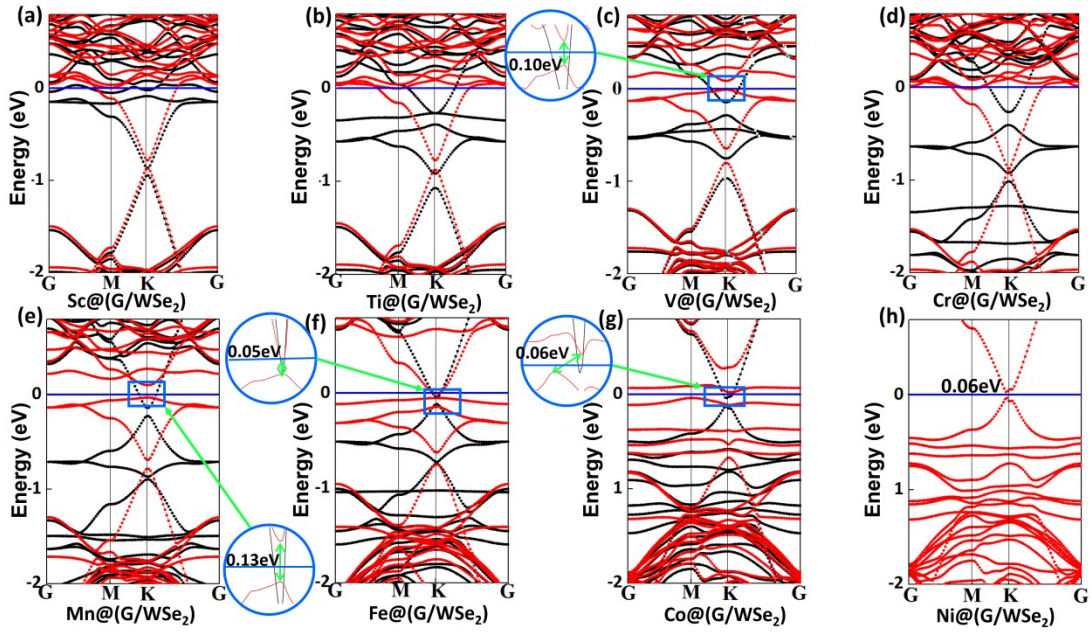

Figure S8. (a-h) Band structures of TM@(G/WSe_2)s, TM=Sc-Ni, respectively. Red and black lines represent the bands of spin up and spin down, respectively.

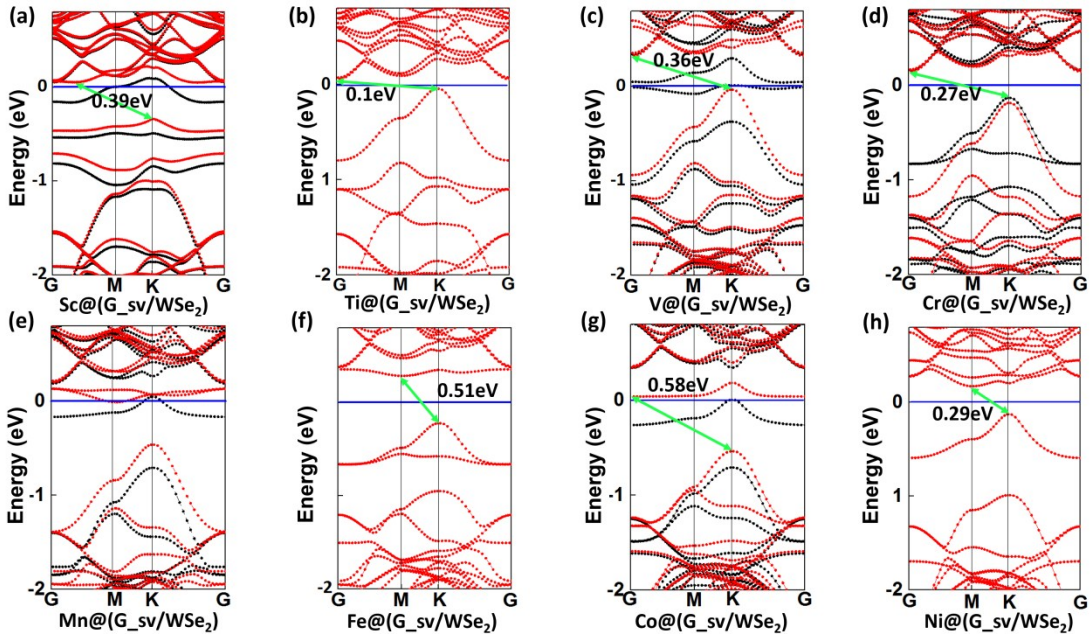

Figure S9. (a-h) Band structures of TM@(G_sv/WSe_2)s, TM=Sc-Ni, respectively. Red and black lines represent the bands of spin up and spin down, respectively.

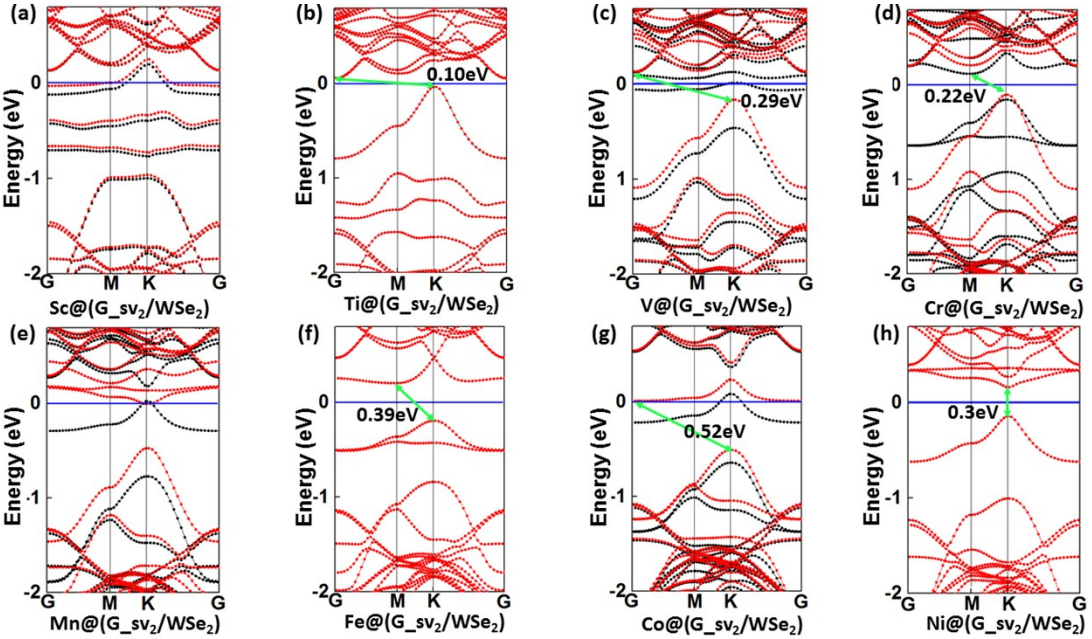

Figure S10. (a-h) Band structures of TM@(G_sv_2/WSe_2)s, TM=Sc-Ni, respectively. Red and black lines represent the bands of spin up and spin down, respectively.

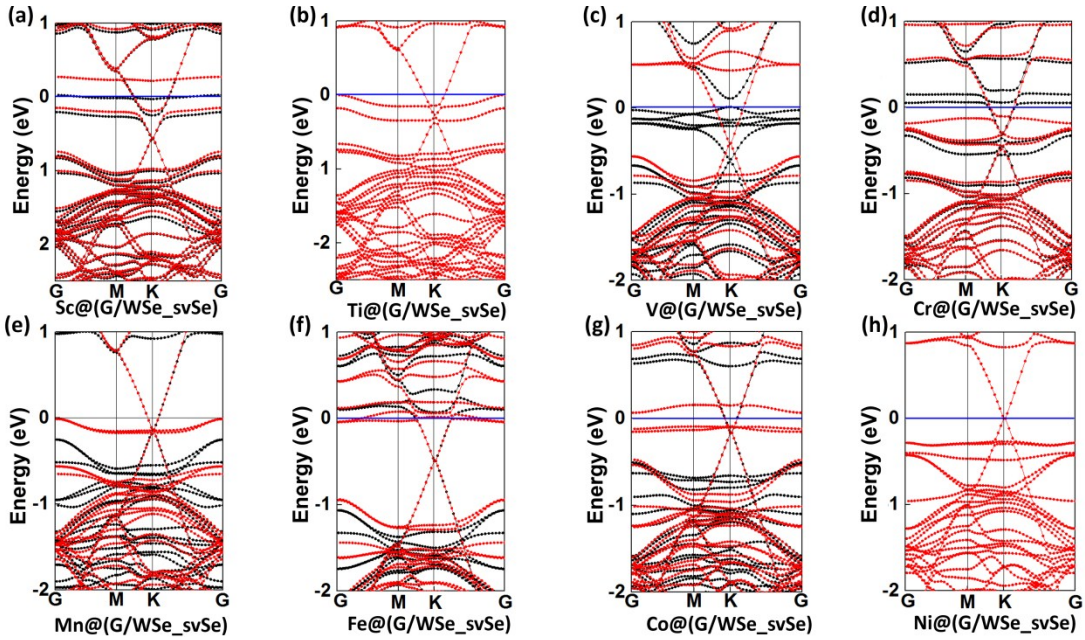

Figure S11. (a-h) Band structures of TM@(G/WSe_svSe)s, TM=Sc-Ni, respectively. Red and black lines represent the bands of spin up and spin down, respectively.