Supporting Information for

Regulating the electronic properties of WGe_2N_4 monolayer by adsorption of 4d transition metal atoms towards spintronic devices

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Table S1. The adsorption energies (E_a), adsorption distances (D), magnetic moments (M) and band gaps (E_{gap}) of the WGe_2N_4 monolayer adsorbing 4d transition metal atoms (Y–Cd) with the most stable adsorption structures.

TM	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
E_a/eV	−2.66	−1.93	−1.6	−0.56	−1.00	−1.80	−1.93	−1.60	−0.49	−0.30
D/Å	1.10	1.78	1.31	2.38	2.16	1.78	1.79	1.90	2.53	3.06
M/μ_B	0.77	3.02	2.90	5.62	4.98	2.01	0.96	0.00	−0.02	0.00
E_{gap}/eV	0.00	0.00	0.00	0.00	0.09	0.12	0.18	0.66	0.00	0.60

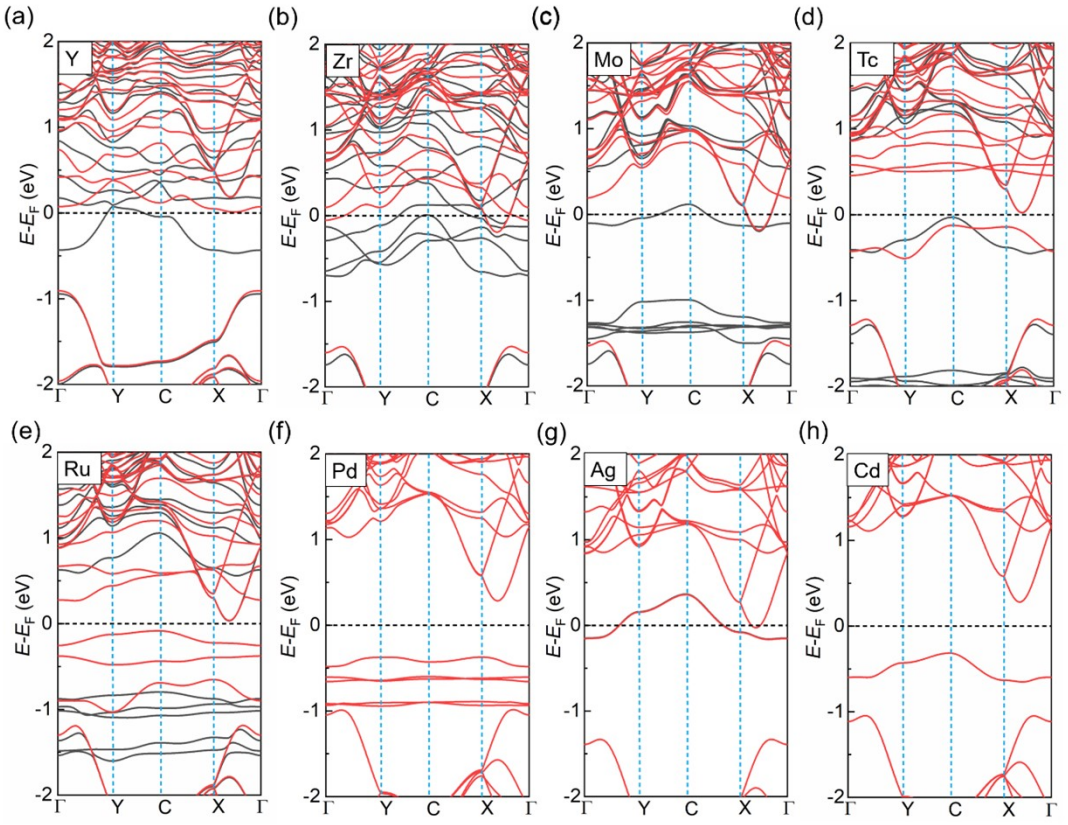

Fig. S1 The band structures of the WGe_2N_4 monolayer with 4d transition metal adatoms (Y, Zr, Mo, Tc, Ru, Pd, Ag, and Cd).

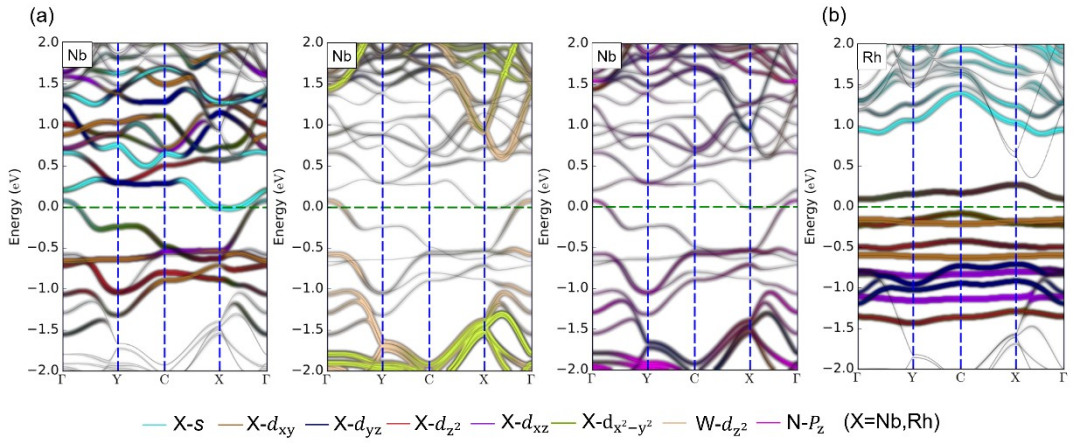

Fig. S2 The orbital projected band structures of the (a) Nb- and Rh-adsorbed WGe_2N_4 monolayer. In order to observe the occupation of the atomic orbitals of the Nb-adsorbed system more clearly, the occupation of the orbitals of Nb, W, and N atoms are plotted separately.

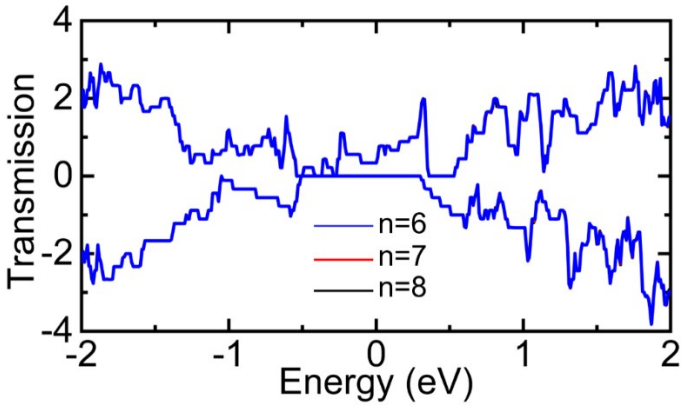

Fig. S3 The zero-bias transmission spectra of Sc-adsorbed WGe_2N_4 device with the central region containing 6, 7, and 8 units with parallel magnetization configuration.