Supporting Information for

Surface engineering of phosphorene nanoribbons by transition metal heteroatoms for spintronics

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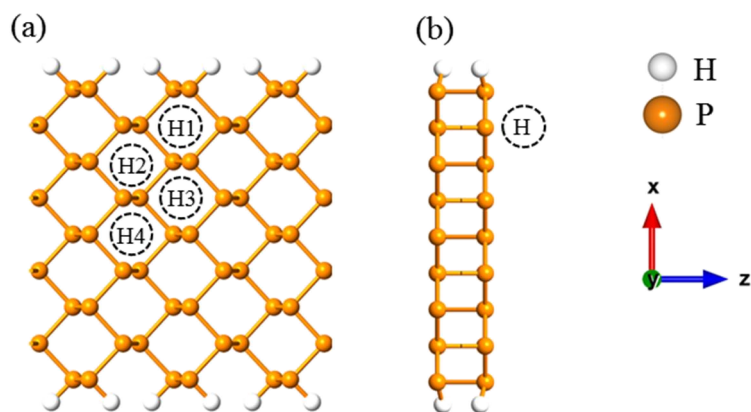

Fig. S1 (a) Top view and (b) side view for structures of H-APNR with 3 unit cells. Here, H1~H4 represent different hollow sites of adsorption for TM atoms.
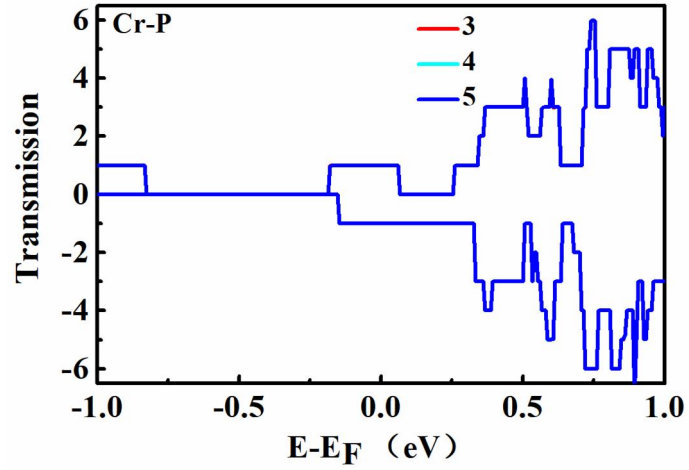
Fig. S2 The transmission spectra of Cr adsorped H-APNRs for central region containing 3, 4, and 5 units with the zero bias in parallel spin configurations.
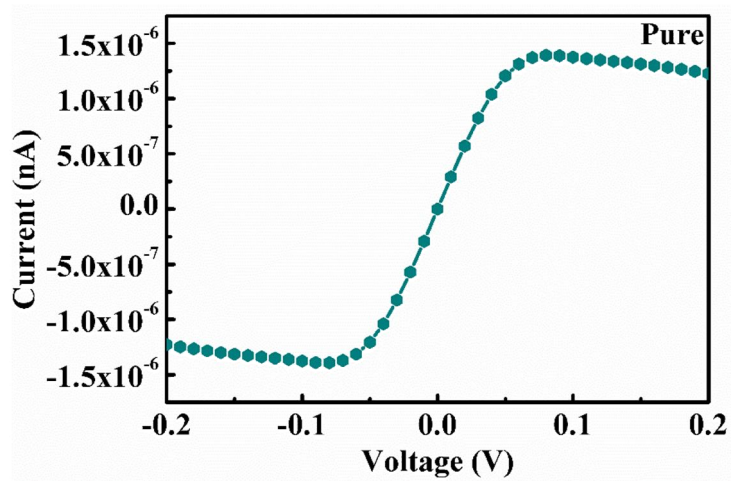

Fig. S3 Current-voltage characteristic curve of pure H-APNR.

Table S1 The maximum displacements of phosphorus atoms in adsorption configurations from the initial locations in phosphene nanoribbons in the y direction (ΔY_{Max}), shortest distances between TM atoms and phosphorus atom(d_{TM-P}), adsorption energy (E_a and E_a^*), cohesive energy (E_c), magnetic moment (M), and the charge transfer (ΔQ) of TM atoms.

Adatom	Site	ΔY_{Max} (Å)	d_{TM-P} (Å)	E_a (eV)	E_a^* (eV)	E_c (eV)	M (μ_B)	ΔQ (e)
Sc	H1	0.31	2.55	-3.46	–		0.71	
	H2	0.26	2.57	-3.45	–		0.76	
	H3	0.29	2.59	-3.46	–		0.74	
	H4	0.28	2.59	-3.46	–	-3.90	0.73	-0.15
Ti	H1	0.38	2.42	-4.10	–		1.82	
	H2	0.29	2.43	-4.08	–		1.89	
	H3	0.30	2.43	-4.15	–		1.89	
	H4	0.30	2.44	-4.16	–	-4.85	1.89	-0.19
V	H1	0.31	2.33	-2.82	–		2.86	
	H2	0.37	2.34	-2.85	–		2.85	
	H3	0.30	2.34	-2.86	–		2.85	
	H4	0.38	2.34	-2.86	–	-5.31	2.84	-0.10
Cr	H1	0.06	2.45	-2.92	–		4.83	
	H2	0.09	2.45	-3.02	–		4.82	
	H3	0.09	2.45	-3.05	–		4.82	
	H4	0.04	2.45	-3.05	–	-4.10	4.82	-0.14
Mn	H1	0.72	2.33	-2.13	-1.20		4.72	
	H2	0.23	2.06	-2.27	-1.57		4.67	
	H3	0.17	2.33	-2.26	-1.57		4.65	
	H4	0.18	2.33	-2.27	-1.59	-2.92	4.65	-0.08
Fe	H1	0.07	2.13	-4.10	-3.06		2.29	
	H2	0.15	2.13	-4.04	-2.61		2.33	
	H3	0.18	2.13	-4.06	-2.94		2.33	
	H4	0.21	2.14	-4.07	-2.81	-4.28	2.34	-0.09
Co	H1	0.09	2.11	-4.99	-3.83		1.09	
	H2	0.24	2.12	-4.95	-3.85		1.04	
	H3	0.16	2.12	-4.98	-3.87		1.04	
	H4	0.16	2.44	-4.99	-3.88	-4.39	1.04	-0.07
Ni	H1	0.31	2.12	-5.30	-4.28		0.00	
	H2	0.26	2.12	-5.29	-4.26		0.00	
	H3	0.11	2.12	-5.32	-4.28		0.00	
	H4	0.08	2.12	-5.33	-4.29	-4.44	0.00	-0.06

E_a^* represents the adsorption energy by the other group[1].

Table S2 The comparisons for the maximum displacements of phosphorus atoms in adsorption configurations from the initial locations in phosphorene nanoribbons in the y direction (ΔY_{Max}), the shortest distances between TM atoms and phosphorus atom (d_{TM-P}), and the adsorption energy (E_a) without (no vdW) and with vdW consideration (vdW).

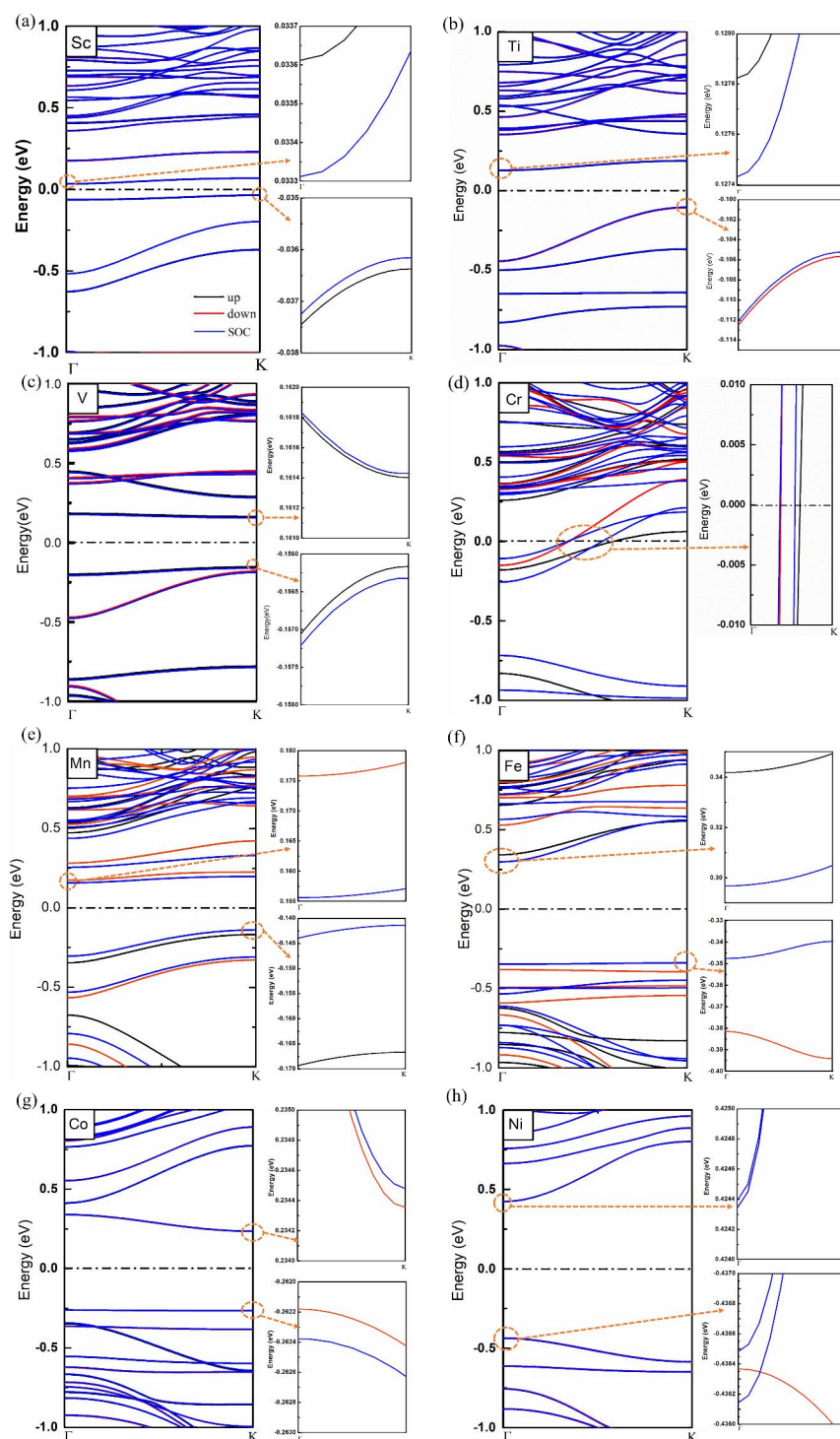| Adatom	ΔY_{Max} (Å)		d_{TM-P} (Å)		E_a (eV)	
	no vdW	vdW	no vdW	vdW	no vdW	vdW
Sc	0.28	0.25	2.59	2.58	-3.46	-3.26
Ti	0.30	0.28	2.44	2.44	-4.16	-4.16
V	0.38	0.37	2.34	2.34	-2.86	-2.86
Cr	0.04	0.05	2.45	2.45	-3.05	-3.05
Mn	0.18	0.21	2.33	2.33	-2.27	-2.26
Fe	0.21	0.21	2.14	2.13	-4.07	-4.06
Co	0.16	0.15	2.44	2.43	-4.99	-5.01
Ni	0.08	0.11	2.12	2.12	-5.53	-5.53

Fig. S4 The band structures of (a) Sc, (b) Ti, (c) V, (d) Cr, (e) Mn, (f) Fe, (g) Co and (h) Ni adsorbed H-APNRs. The black, red and blue colors show the band structure of spin up, down and the spin-orbit coupling, respectively..

1.   Y.-C. Rao, P. Zhang, S.-F. Li, X.-M. Duan and S.-H. Wei, *Phys. Chem. Chem. Phys.*, 2018, **20**, 12916–12922.