

Supporting Information for

**Modulating the electronic structures of blue phosphorene towards spintronics**

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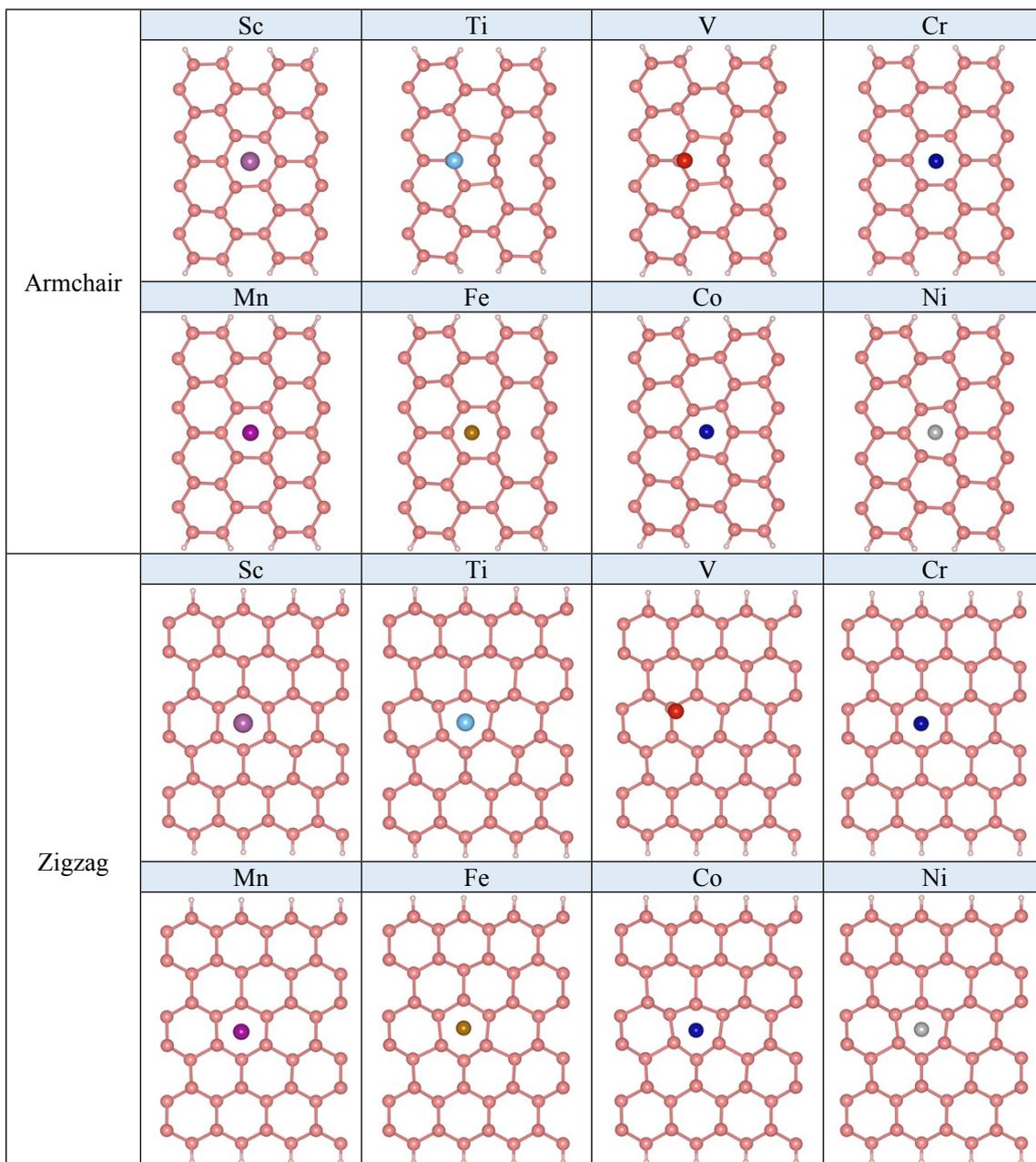


Fig. S1 The relaxed geometrical structures of X@H-APNRs and H-ZPNRs (X=Sc, Ti, V, Cr, Mn, Fe, Co, and Ni).

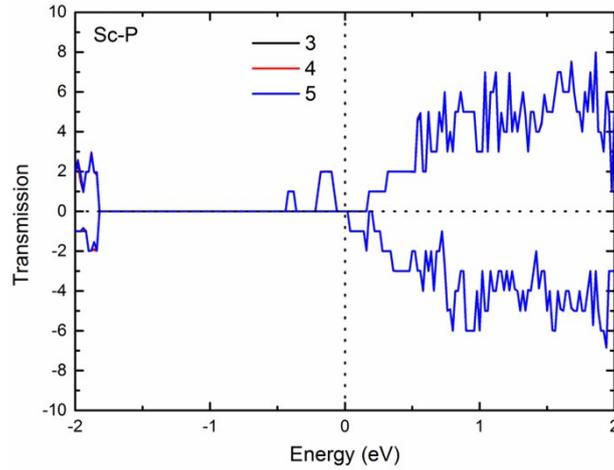


Fig. S2 The equilibrium transmission spectra of Sc-adsorbed nanoribbons with scattering region containing 3, 4 and 5 units of cell with P spin configuration.

Table S1 The minimum distance between TM atoms and blue phosphorene  $D_{M-P}$  (Å), adsorption energy  $E_a$ ,  $E_a^{(1)}$  and  $E_a^{(2)}$  (the unit is eV) of transition metal adatoms on blue phosphorene nanoribbon, black phosphorene nanoribbon, and graphene nanoribbon, and experimental cohesive energies per atom of bulk metals  $E_c$  (eV) and the magnetic moments  $M$  ( $\mu_B$ ).

M	Type	$D_{M-P}$	$E_a$	$E_a^{(1)}$	$E_a^{(2)}$	$E_c$	$M$
Sc	Arm.	2.55	-2.43	-3.46	---	-3.90	1.30
	Zig.	2.55	-2.43	---	---		1.30
Ti	Arm.	2.47	-3.92	-4.16	-1.99	-4.85	1.86
	Zig.	2.50	-3.32	---	---		2.23
V	Arm.	2.34	-2.57	-2.86	---	-5.31	2.80
	Zig.	2.34	-2.41	---	---		3.46
Cr	Arm.	2.58	-2.71	-3.05	-0.25	-4.10	4.96
	Zig.	2.57	-2.72	---	---		4.95
Mn	Arm.	2.48	-1.67	-2.27	-0.07	-2.92	4.77
	Zig.	2.49	-1.66	---	---		4.79
Fe	Arm.	2.20	-2.95	-4.07	-0.94	-4.28	2.71
	Zig.	2.17	-2.95	---	---		2.52
Co	Arm.	2.18	-4.14	-4.99	-1.08	-4.39	1.20
	Zig.	2.18	-4.12	---	---		1.20
Ni	Arm.	2.17	-4.60	-5.33	---	-4.44	0
	Zig.	2.17	-4.60	---	---		0

Table S2 The adsorption sites, adsorption energy  $E_a$  and separation distance  $d_{Co-Co}$  involved in the growth pattern.

Co@H-APNR	Sites	$E_a$ (eV)	$d_{Co-Co}$ (Å)
	H1+H4	-4.10	4.86
	<b>H2+H4</b>	<b>-4.59</b>	<b>2.41</b>
	<b>H3+H4</b>	<b>-4.58</b>	<b>2.47</b>
	H4+H4	-4.19	5.65
	H3+H3+H4 (tetrahedron)	-4.91	2.41
	<b>H3+H3+H4+H4</b>	<b>-5.10</b>	<b>2.42</b>

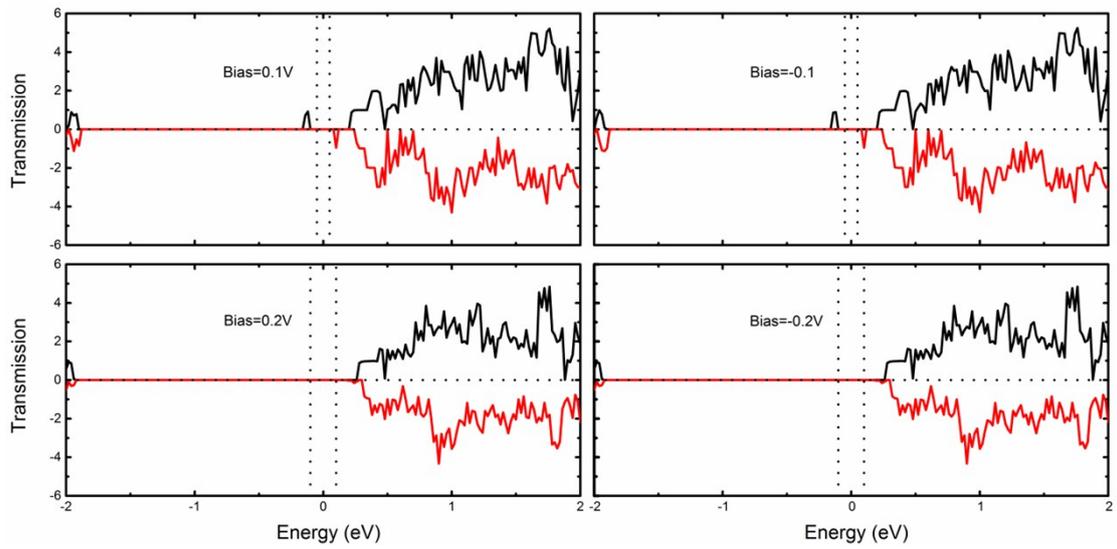


Fig. S3 Transmission spectra of Sc@H-ZPNR with P configuration at  $\pm 0.1$  V and  $\pm 0.2$  V.