Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Schottky diodes based on blue phosphorus nanoribbon homojunctions

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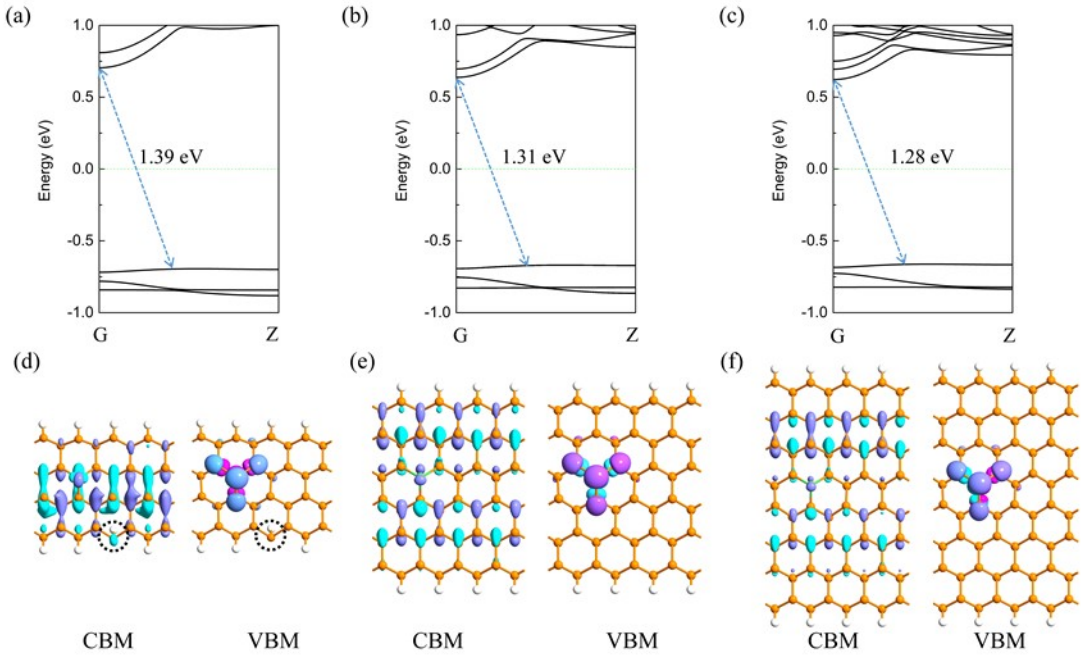

Fig. S1 (a)–(c) The energy band structures and (d)–(f) Bloch states of the Ni-adsorbed H-ZPNR with different widths. The isovalues are fixed as 0.07 e Bohr^{-3} for all Bloch states.

Table1 Adsorption energies of the transition metal atoms on the top site of the H-ZPNR

Transition metal adsorption atom	E_a (eV)
Sc	−3.04
Ti	−3.59
V	−2.42
Cr	−2.77
Mn	−2.25
Fe	−3.96
Co	−4.86
Ni	−5.15

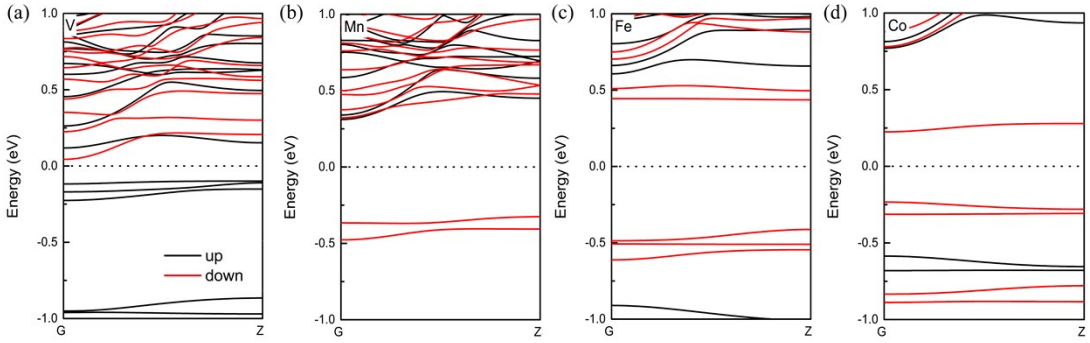

Fig. S2 The band structures of (a) V, (b) Mn, (c) Fe, and (d) Co adsorbed H-ZPNR.

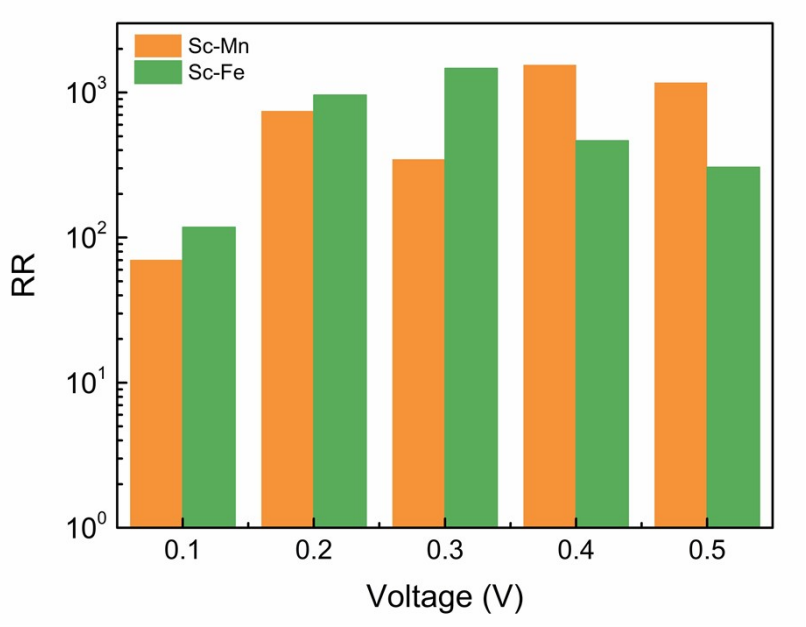

Fig. S3 Rectification ratios of the Sc–Mn and Sc–Fe devices.

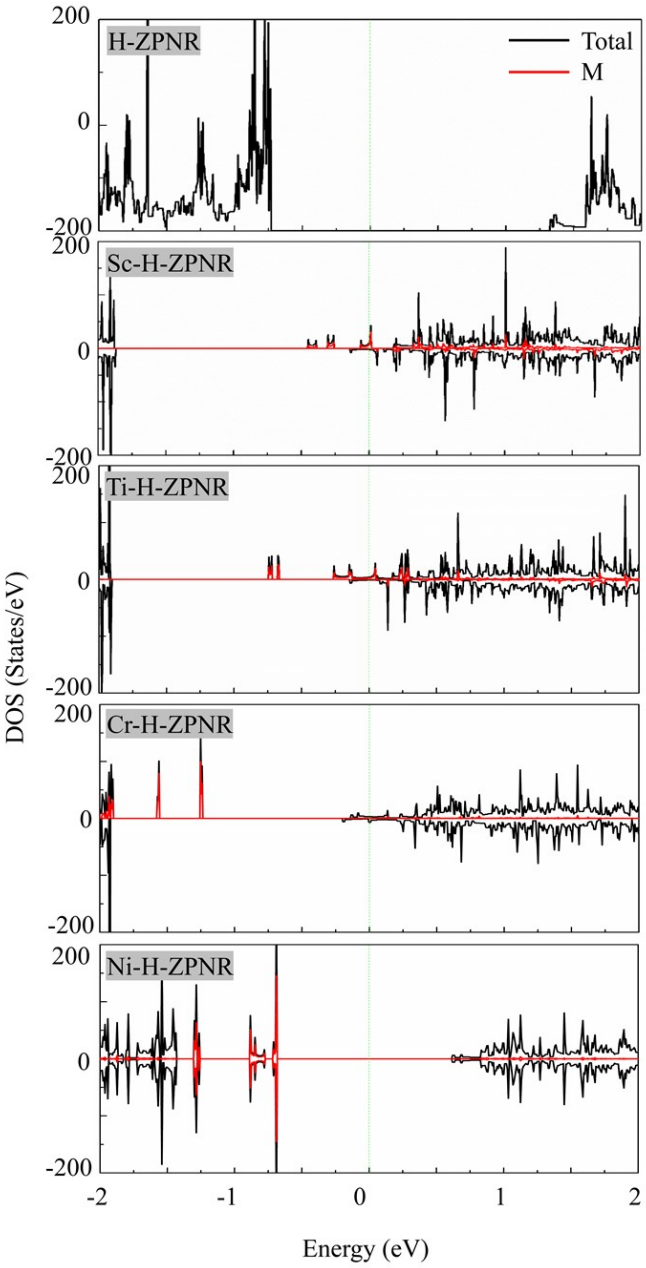

Fig. S4 The projected density of states (PDOS) for H-ZPNR and Sc, Ti, Cr, and Ni adsorbed H-ZPNR.

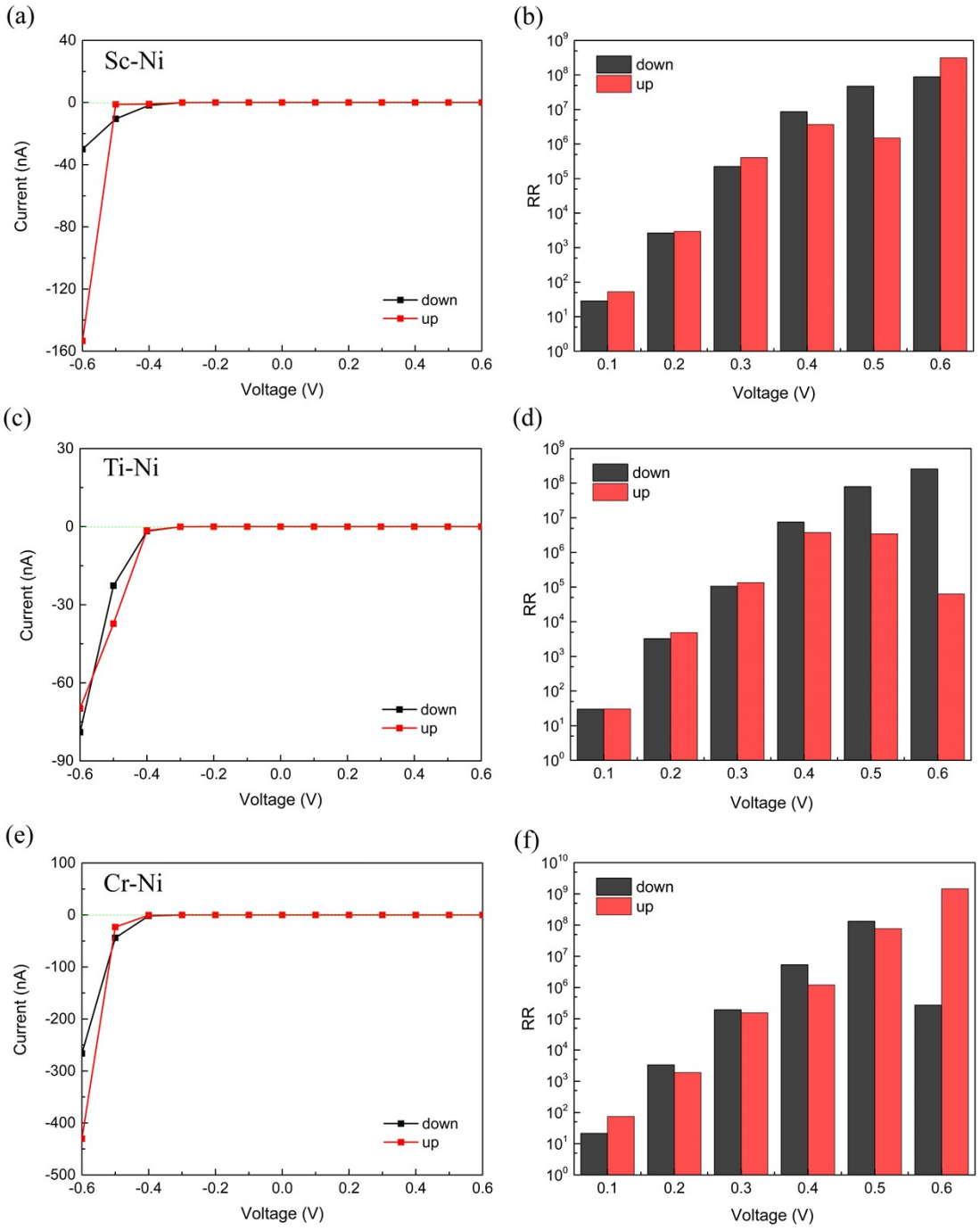

Fig. S5 Spin-dependent *I-V* curves and *RR* of (a)–(b) Sc–Ni, (c)–(d) Ti–Ni, and (e)–(f) Cr–Ni homojunction devices, respectively.