Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information

First-Principles Calculations of Inorganic Metallocene Nanowires

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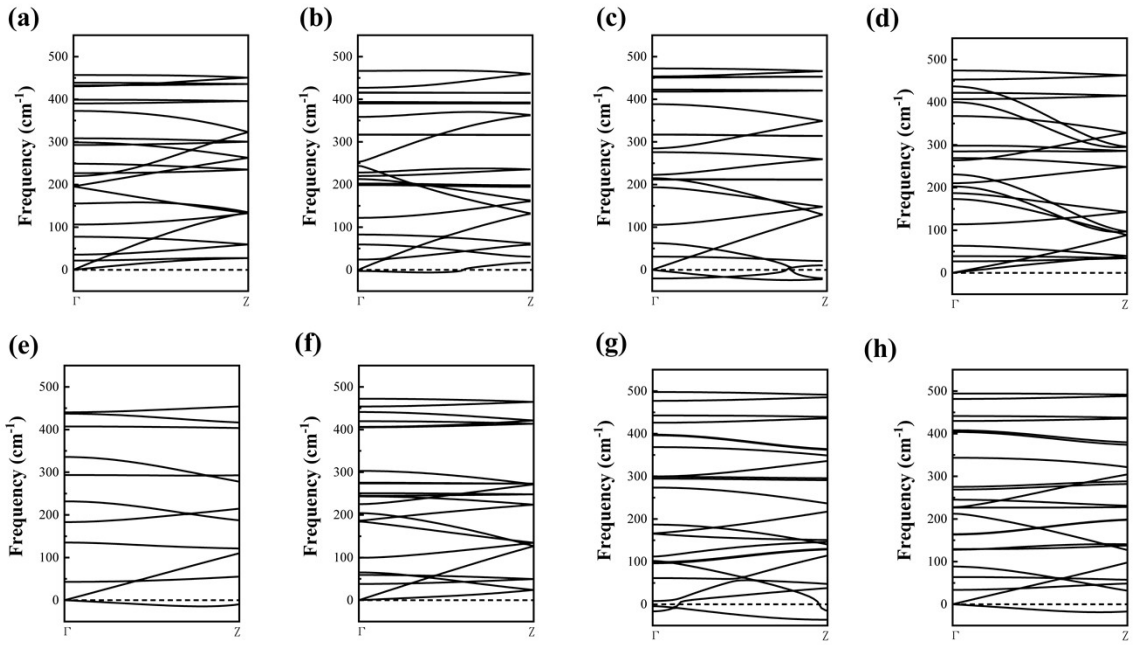

Fig. S1. The calculated phonon dispersion spectra for the lowest energy structures of (a) ScP_4 (b) TiP_4 (c) VP_4 (d) CrP_4 (e) MnP_4 (f) FeP_4 (g) CoP_4 (h) NiP_4 in either Q-type or A-type.

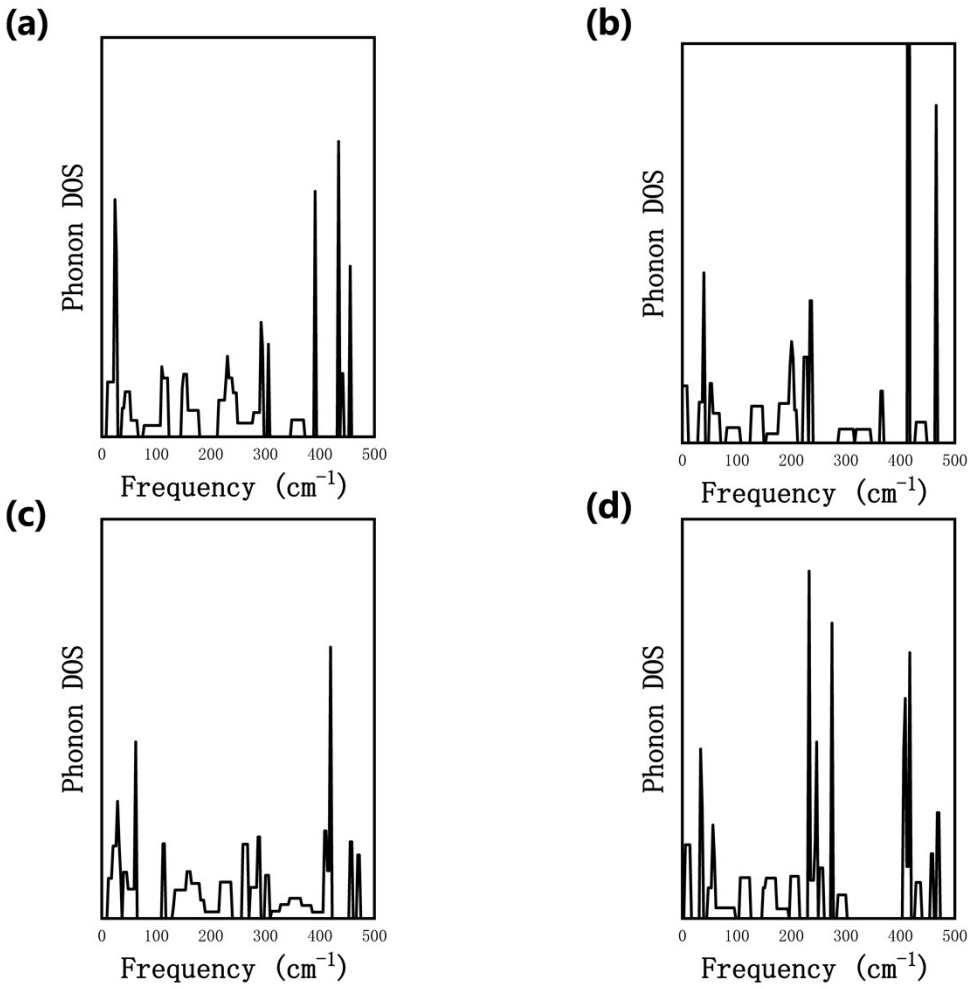

Fig. S2. The phonon density of states of (a) ScP_4 (b) TiP_4 (c) CrP_4 (d) FeP_4 in either Q-type or A-type.

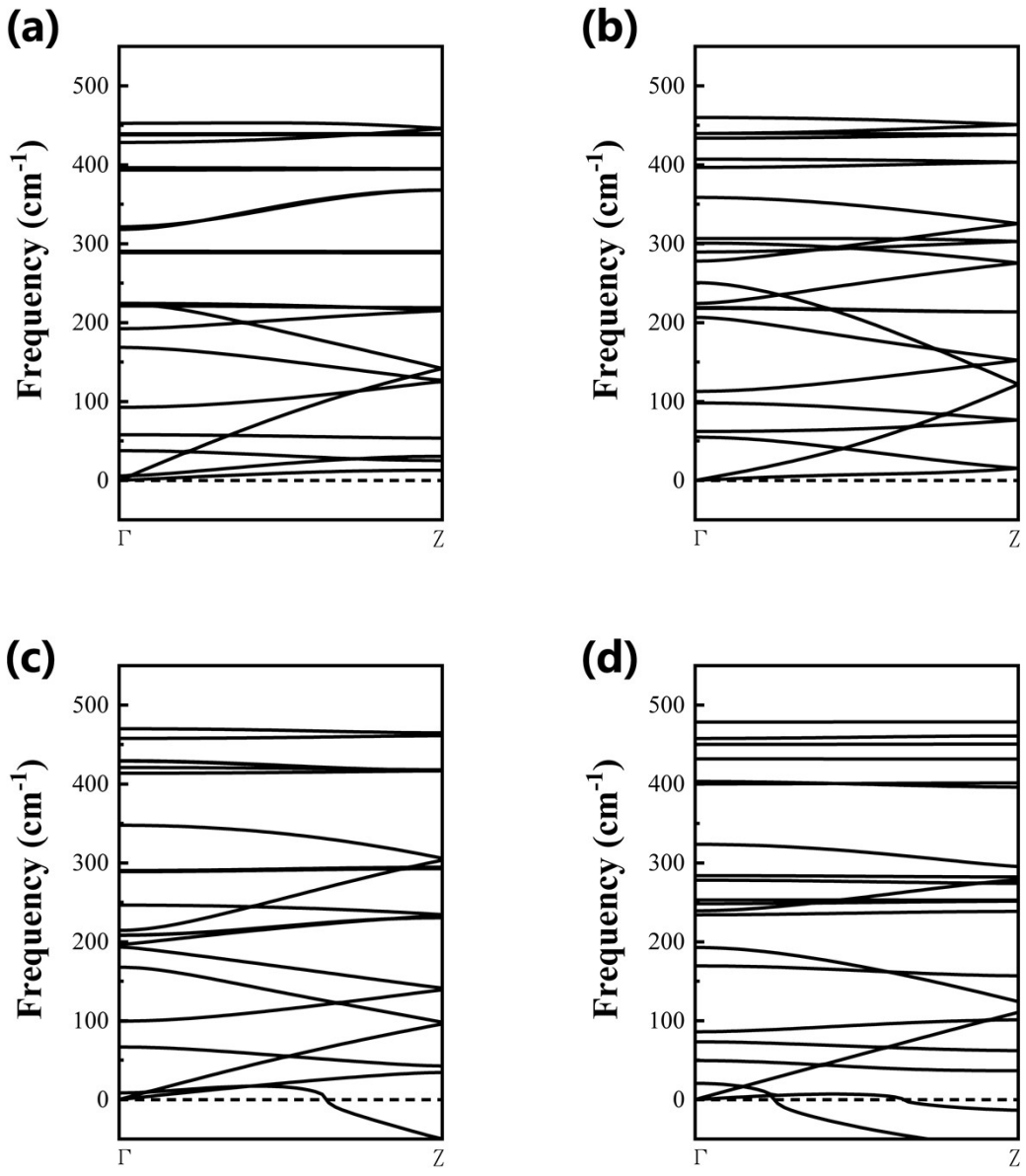

Fig. S3. The calculated phonon dispersion spectra of (a) ScP_4 in A-type (b) TiP_4 in Q-type (c) CrP_4 in A-type (d) FeP_4 in A-type.

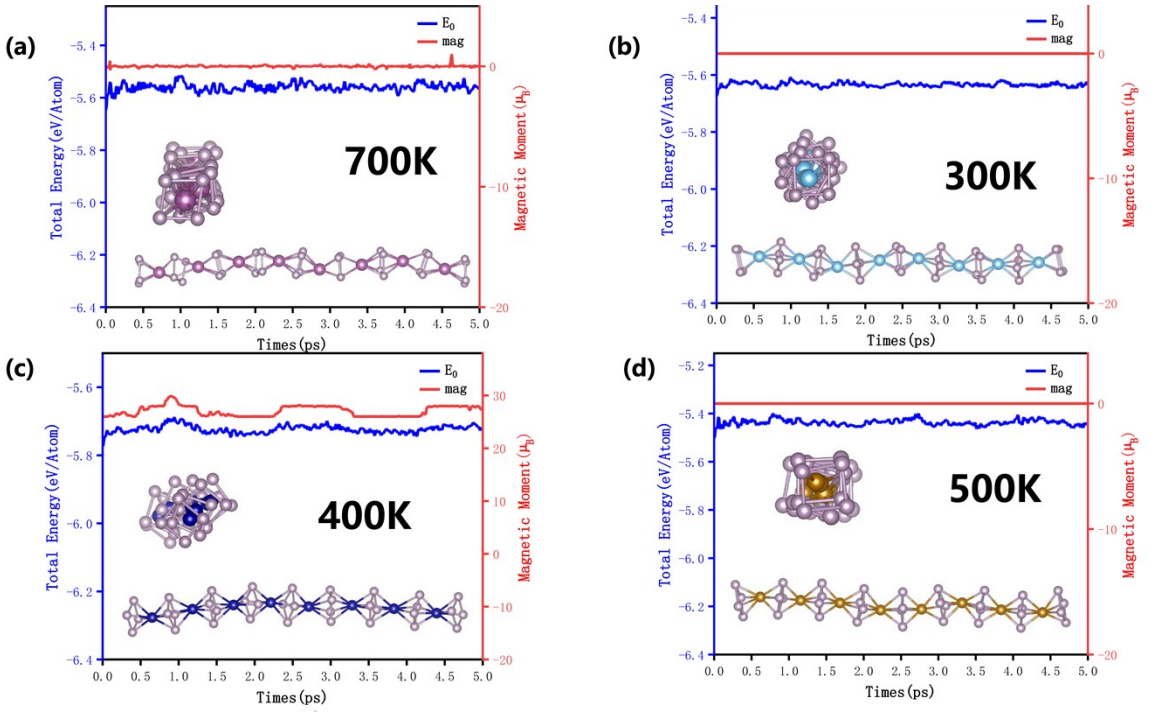

Fig. S4. The evolvement of total energy per atom (E_0, eV/atom) and total magnetic moments (mag, μB) along with time, and the structural snapshot of AIMD simulation for (a)ScP_4 (b)TiP_4 (c)CrP_4 (d)FeP_4.

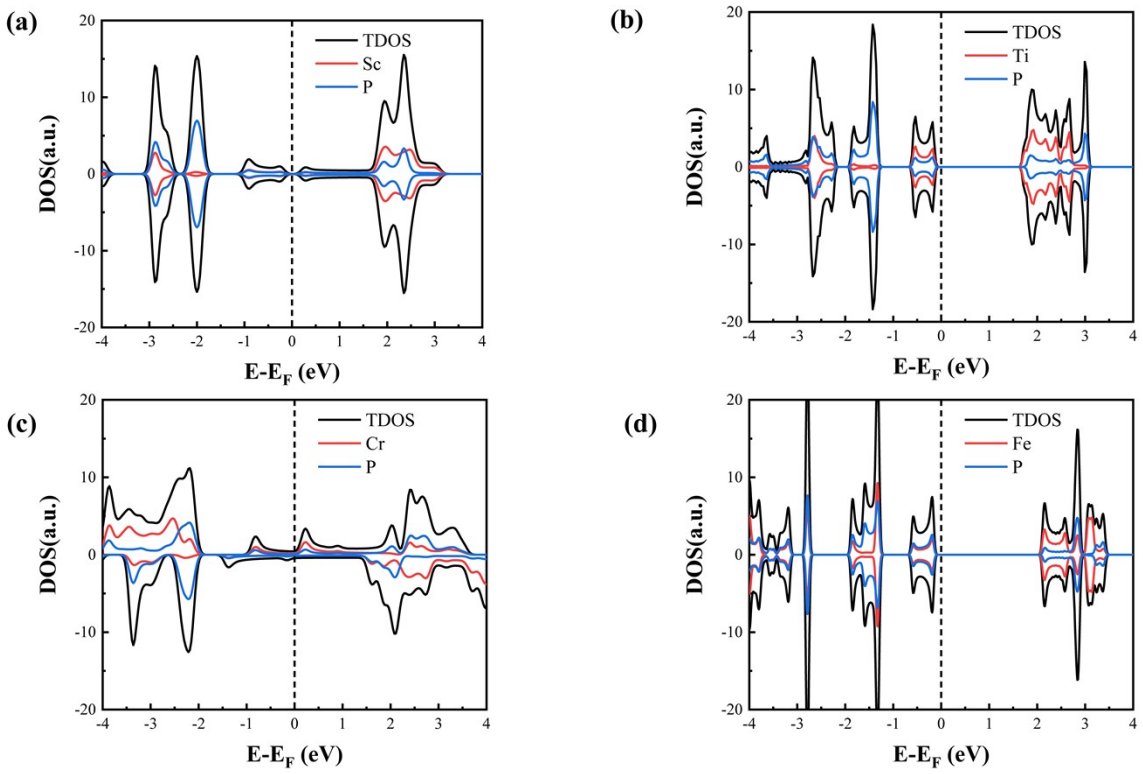

Fig. S5. The calculated total density of states for (a)ScP_4 (b)TiP_4 (c)CrP_4 (d)FeP_4.

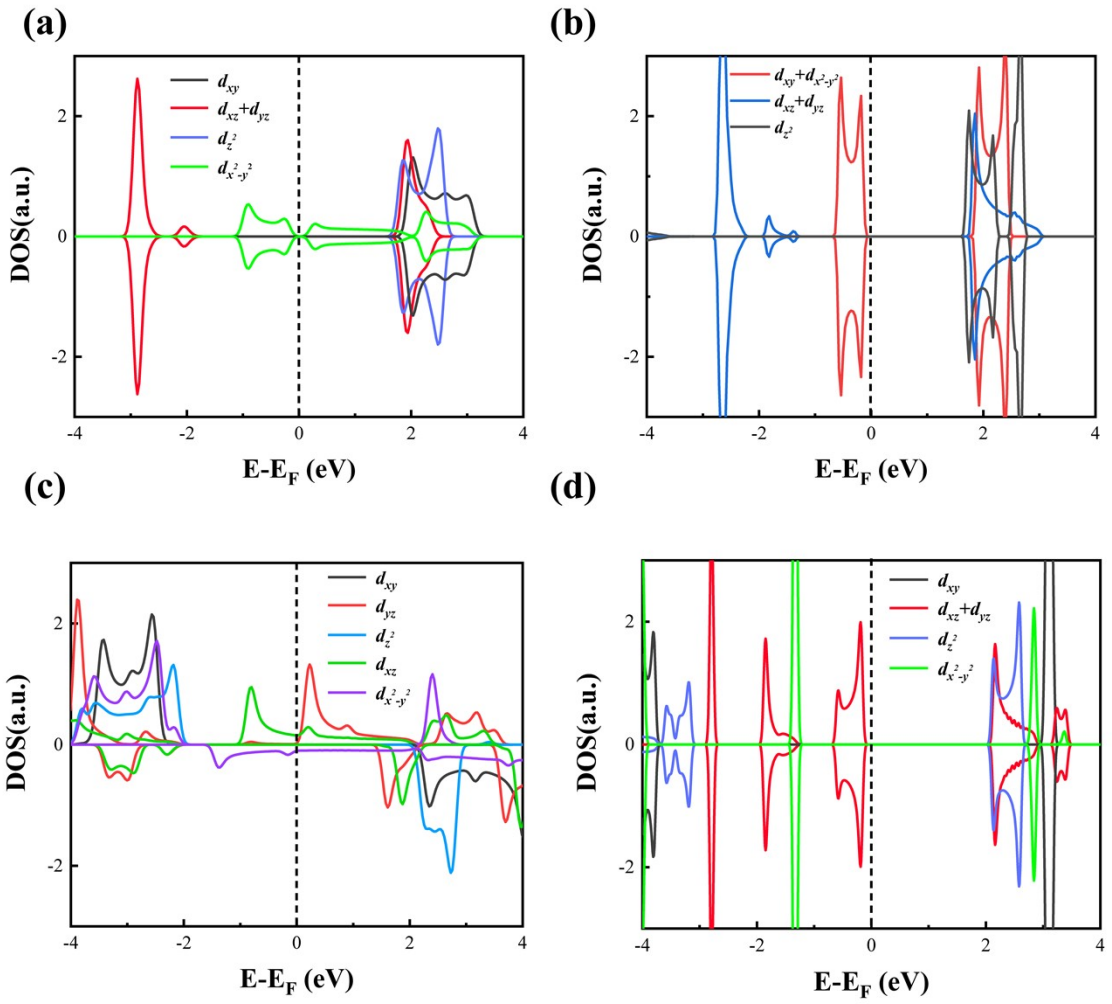

Fig. S6. The calculated local density of states projected on d orbitals of metal for (a)ScP_4 (b)TiP_4 (c)CrP_4 (d)FeP_4.

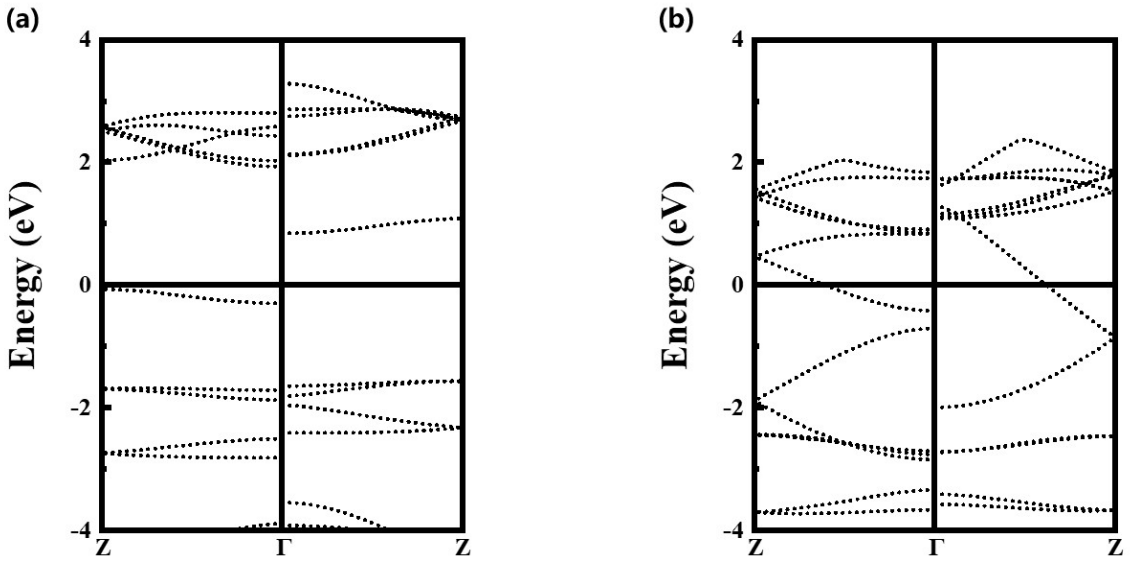

Fig. S7. The electronic band structures for (a) ScP_4 in A-type (b) TiP_4 in Q-type.

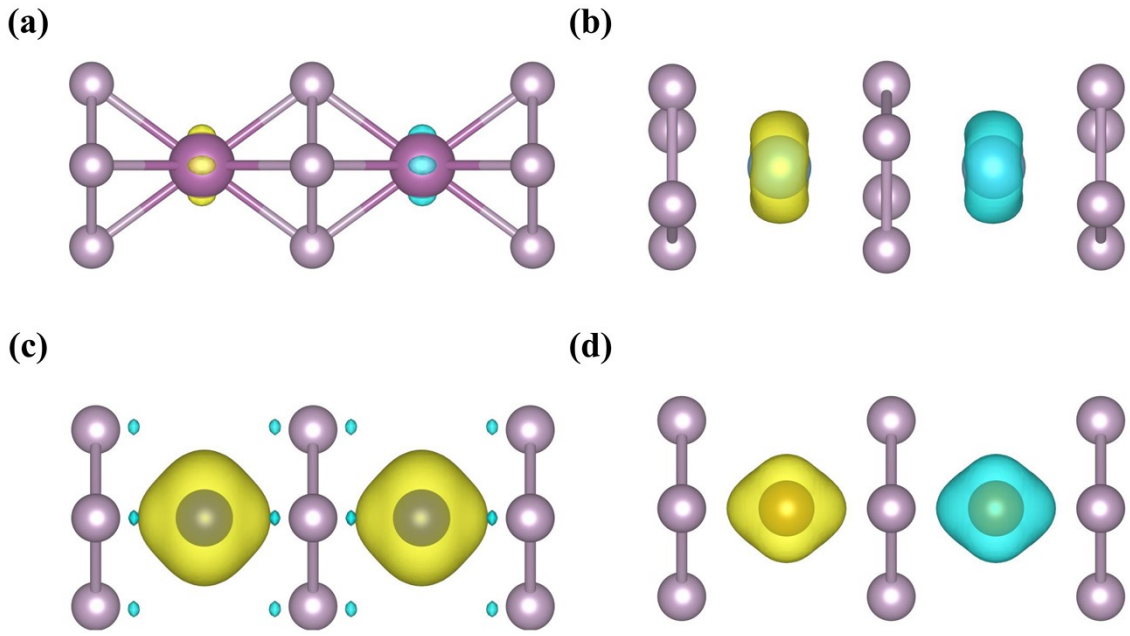

Fig. S8. The spin charge density for (a)ScP_4 (b)TiP_4 (c)CrP_4 (d)FeP_4. The yellow and cyan colours indicate the different spin directions of the electrons, respectively. The isosurface leve is 0.01 $Bohr^{-3}$.

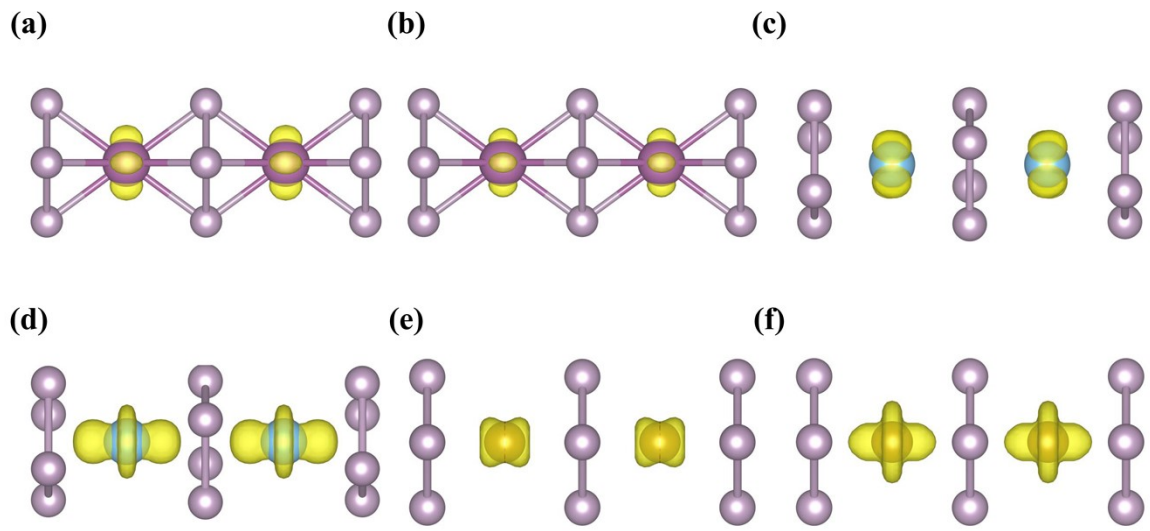

Fig. S9. The band decomposed charge density for (a) VBM at Z for ScP_4 (b) CBM at Z for ScP_4 (c) VBM at Z for TiP_4 (d) CBM at Γ for TiP_4 (e) VBM at Γ for FeP_4 (f) CBM at Γfor FeP_4. The isosurface leve is 0.01 $Bohr^{-3}$.

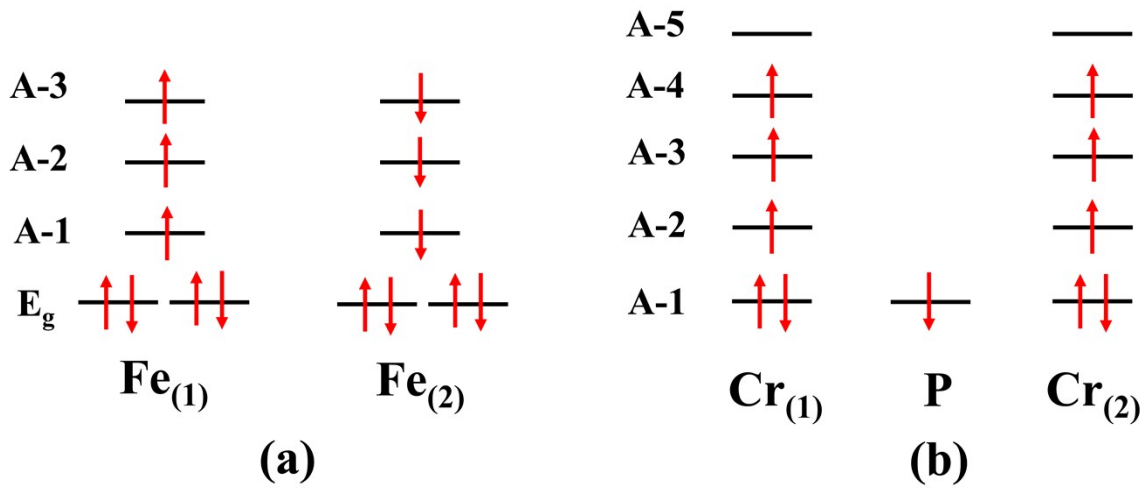

Fig. S10. The electronic configuration of metal atom in FeP_4 and CrP_4 nanowires.

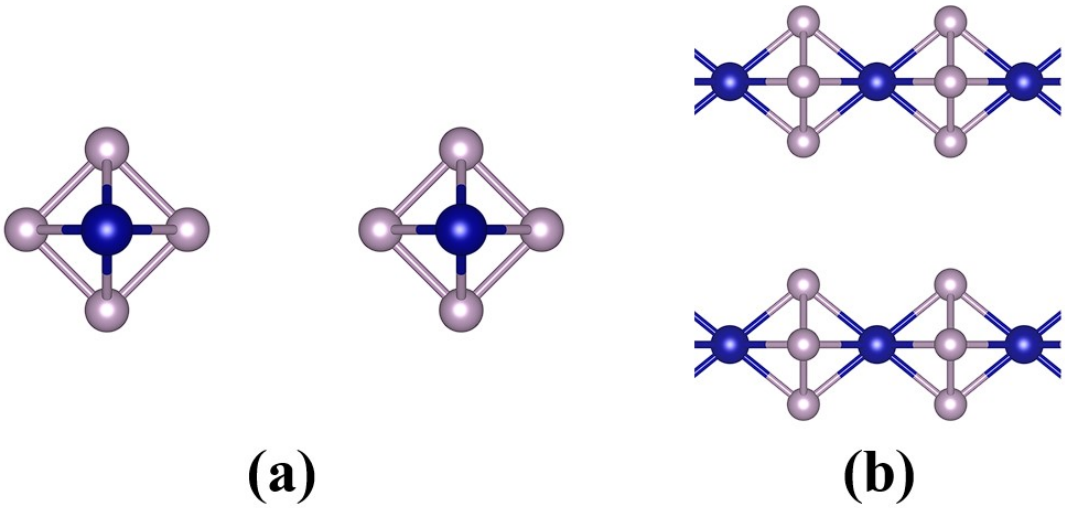

Fig. S11. Structural modeling of CrP_4 interchain coupling model of (a) Front view (b) Top view

Supporting Tables

Table S1. PBE+U was used for structural testing, and the results of the AFM (NM for A-typed ScP_4) and FM (NM for TiP_4) energies regarding to the A-typed and Q-typed structures of MP_4. The energies (eV) given in the table are the difference between the energy of each structure and the energy of the lowest energy structure. ΔE (eV) is defined as the energy difference between the MP_4 nanowire (NW) in Q-type or A-type in the same magnetic ground state per unit cell.

	A-typed AFM MP_4 NW	A-typed FM MP_4 NW	Q-typed AFM MP_4 NW	Q-typed FM MP_4 NW	ΔE
ScP_4	0.759	0.634	0	0.004	0.759
TiP_4	0	0.047	0.378	0.176	0.378
VP_4	0	0.531	0.091	0.674	/
CrP_4	0.772	0.196	0.586	0	0.196
MnP_4	0.594	0.338	0.641	0	/
FeP_4	0.496	0.665	0	0.140	0.496
CoP_4	0.084	0	0.445	0.178	/
NiP_4	0	0.014	0.262	0.364	/

Table S2. Structural information of MP_4 (M = Sc, Ti, Cr and Fe).

	Lattice(Å)	Symmetry Group
ScP_4	8.70	P4/m
TiP_4	7.90	P4/m
CrP_4	7.82	P4/mmm
FeP_4	7.55	P4/mmm

Table S3. The energy per transition metal atom (μeV/atom) relative to the total energy with magnetization direction parallel to easy axis.

	E_{001}(eV)	E_{100}(eV)	$E_{100-001}$(μeV/atom)
ScP_4	-56.52223	-56.52223	0.18
TiP_4	-56.77262	-56.77265	-13.58
CrP_4	-57.81177	-57.81193	-77.86
FeP_4	-55.04702	-55.04637	326.18