Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information for

Ferromagnetic and half-metallic phase transition by doping in one-dimensional narrow-bandgap semiconductor W_6PCl_{17}

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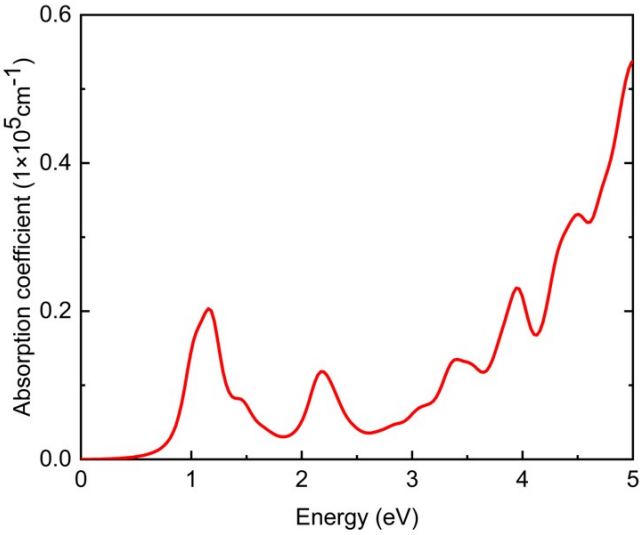

Fig. S1. (a) Calculated absorption spectrum of 1D single-chain W_6PCl_{17} at the HSE06 level with the polarization direction along the chain direction.

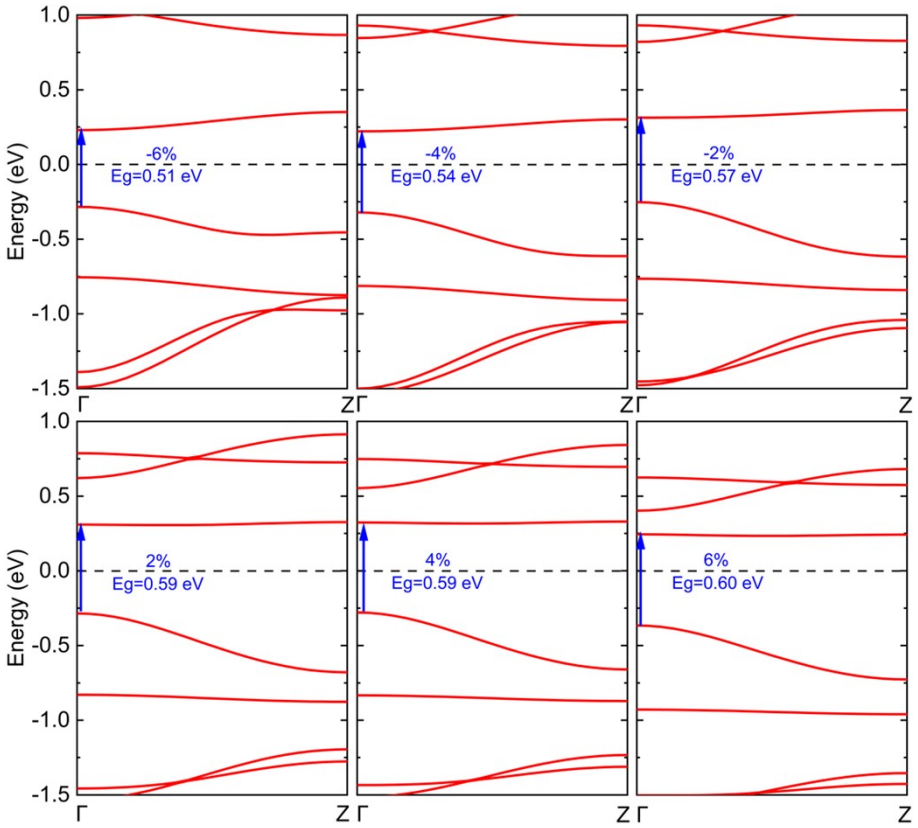

Fig. S2. (a) Electronic band structures of 1D single-chain W_6PCl_{17} under the strains varying from -6% to 6% along the z directions. The band gaps are highlighted in blue. The Fermi level is set at zero.

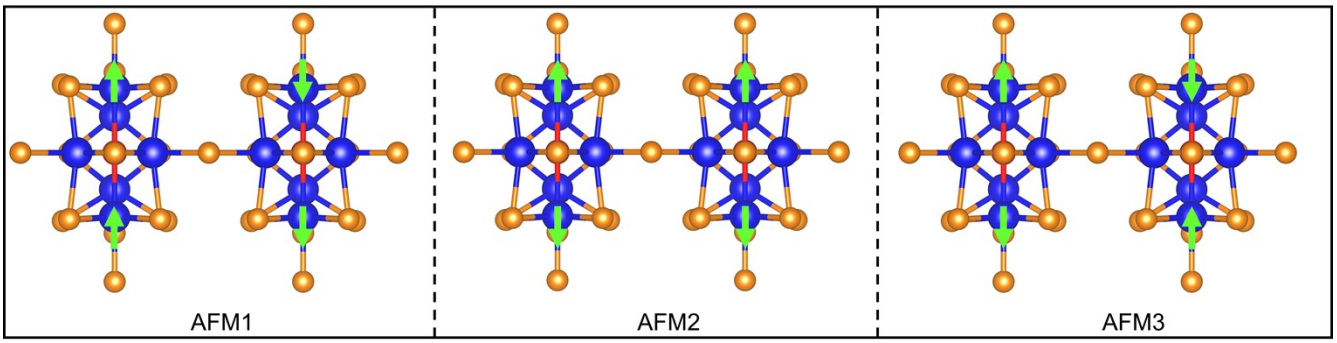

Fig. S3. Possible doping AFM configurations of 1D single-chain W_6PCl_{17}: AFM1, AFM2, and AFM3.

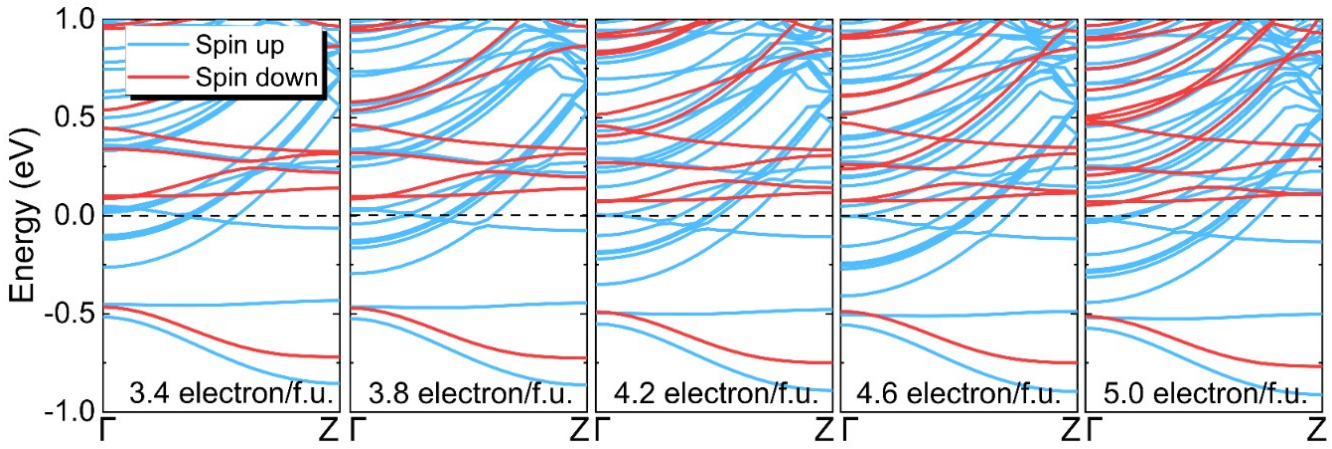

Fig. S4. The spin-polarized band structures of single-chain W_6PCl_{17} calculated with the PBE functional at different electron concentrations *n*: 3.4, 3.8, 4.2, 4.6, and 5.0 electron/f.u., which correspond to 5.17×10^{14}/cm^2, 5.78×10^{14}/cm^2, 6.38×10^{14}/cm^2, 6.99×10^{14}/cm^2, and 7.60×10^{14}/cm^2, respectively. The blue and red solid lines denote the spin-up and spin-down components, respectively.

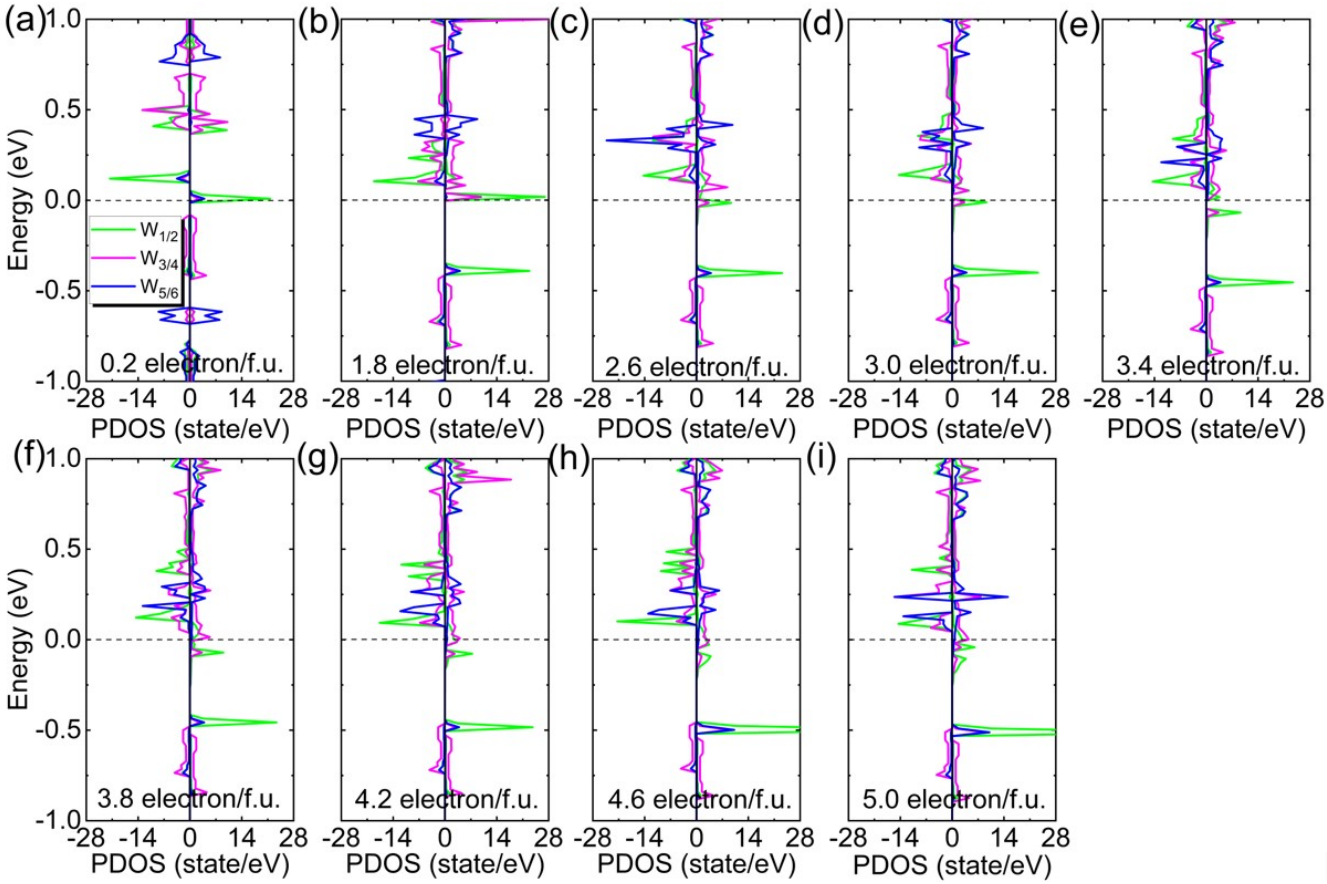

Fig. S5. The PDOS of single-chain W_6PCl_{17} projected onto *d* orbitals of six W atoms in the primitive cell at different electron concentrations: 0.2, 1.8, 2.6, 3.0, 3.4, 3.8, 4.2, 4.6, and 5.0 electron/f.u., which correspond to 0.3×10^{14}/cm^2, 2.74×10^{14}/cm^2, 3.95×10^{14}/cm^2, 4.56×10^{14}/cm^2, 5.17×10^{14}/cm^2, 5.78×10^{14}/cm^2, 6.38×10^{14}/cm^2, 6.99×10^{14}/cm^2, and 7.60×10^{14}/cm^2, respectively.