

Supplementary Materials for “Robust half-metallicities and perfect spin transport properties in 2D transition metal dichlorides”

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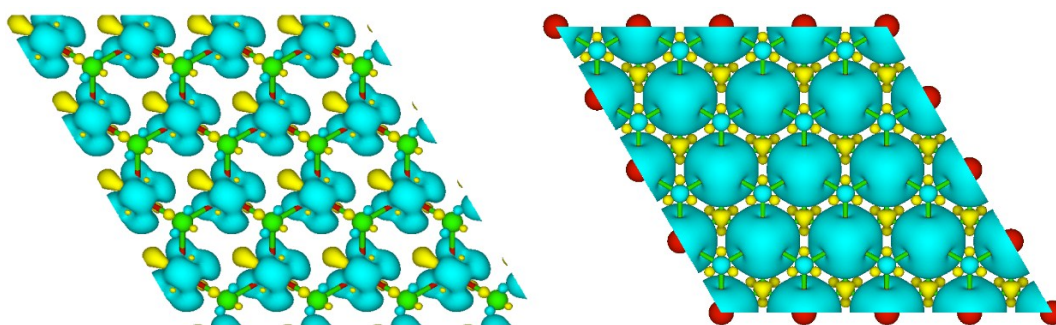
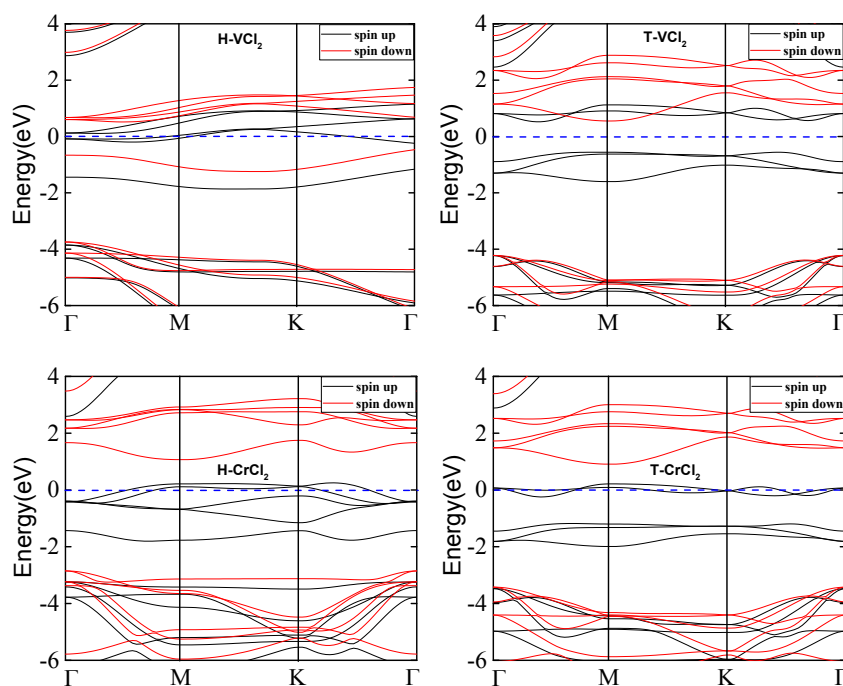


Fig. S1 The spin density isosurface plots (keeping the same value of $0.0026 e/\text{\AA}^3$ for both plots) for (a) 1H-VCl₂ monolayer and (b) 1T-VCl₂ monolayer. The cyan and yellow isosurfaces represent the spin-up and spin-down components, respectively.



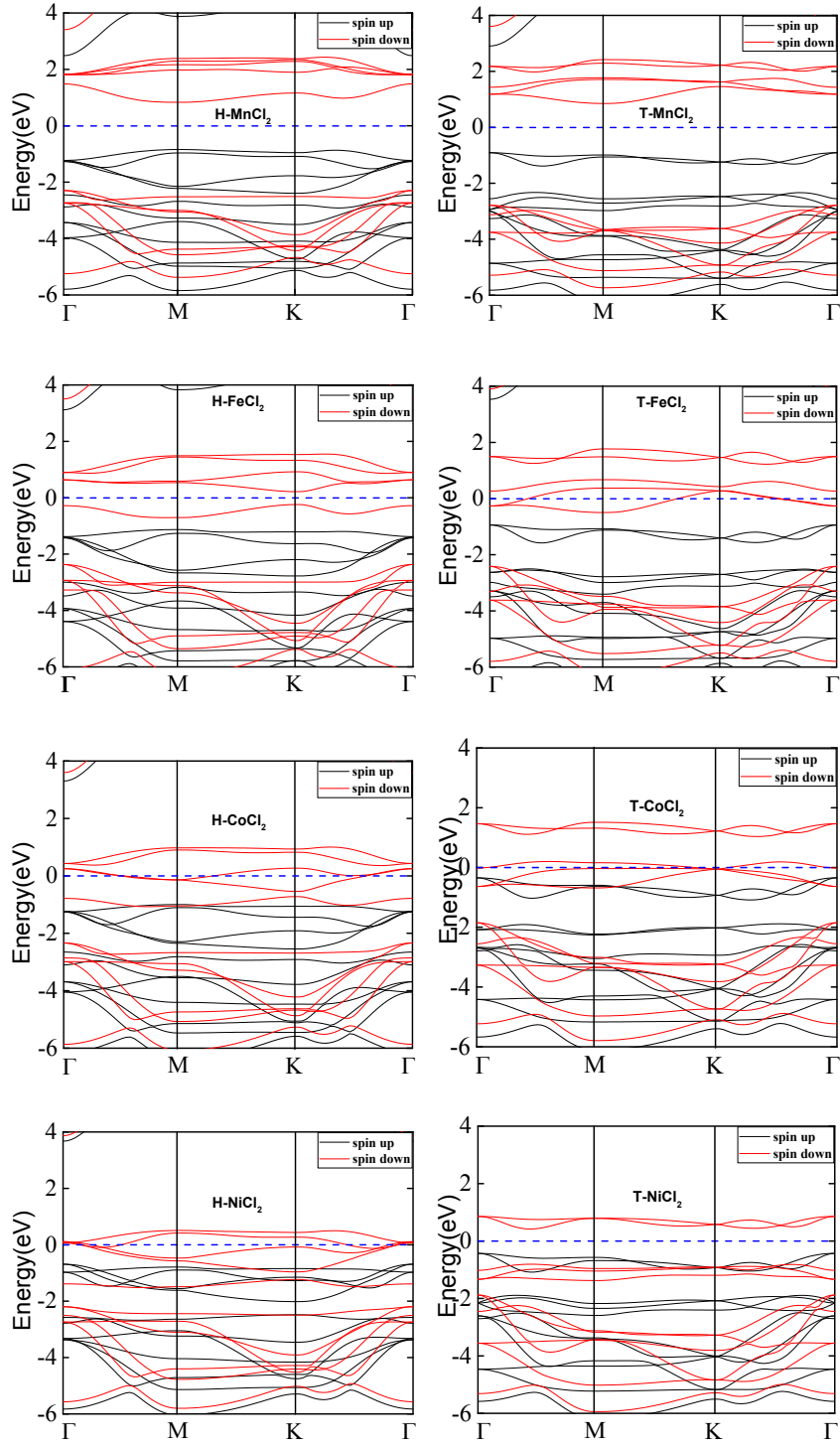
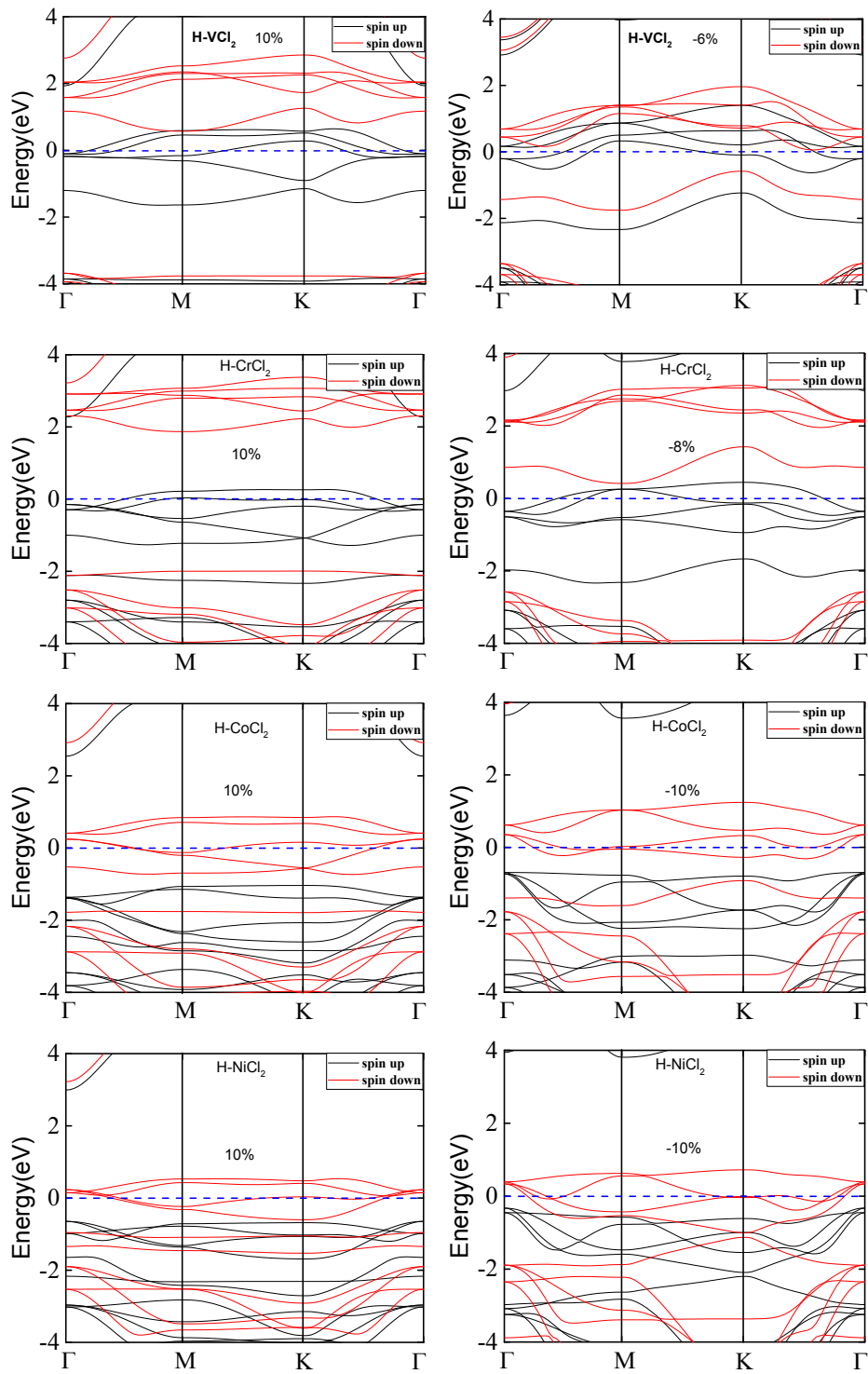


Fig. S2 The calculated spin-dependent band structures of 1H- and 1T-MCl₂ monolayers at equilibrium lattice constants. The dashed line indicates the Fermi level at zero eV.



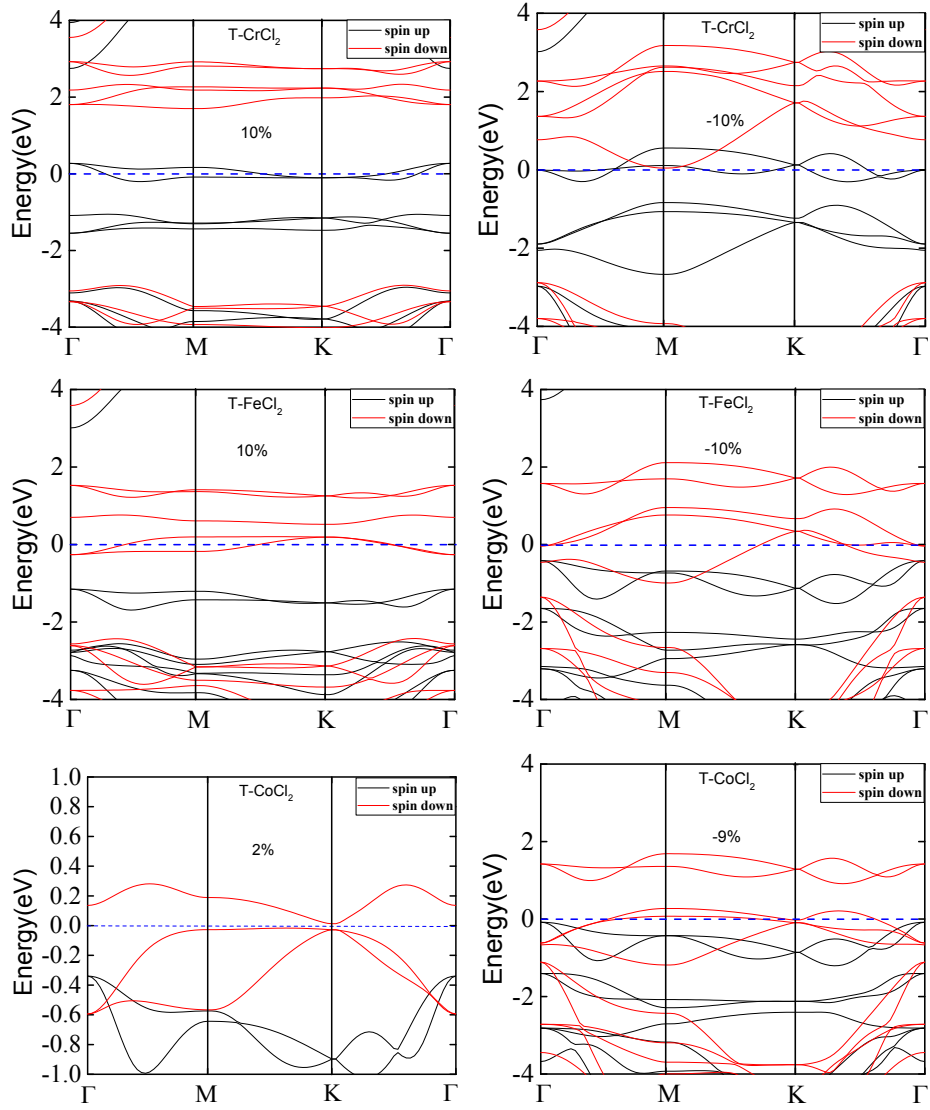


Fig. S3 The calculated spin-dependent band structures of half-metallic 1H-VCl₂, CrCl₂, CoCl₂ and NiCl₂ monolayers as well as 1T-CrCl₂, FeCl₂ and CoCl₂ monolayers at biaxial strains. The dashed line indicates the Fermi level at zero eV.