The Supplemental Material for "Robust bipolar magnetic semiconductors in one-dimensional nanowires of transition metal dihalide"

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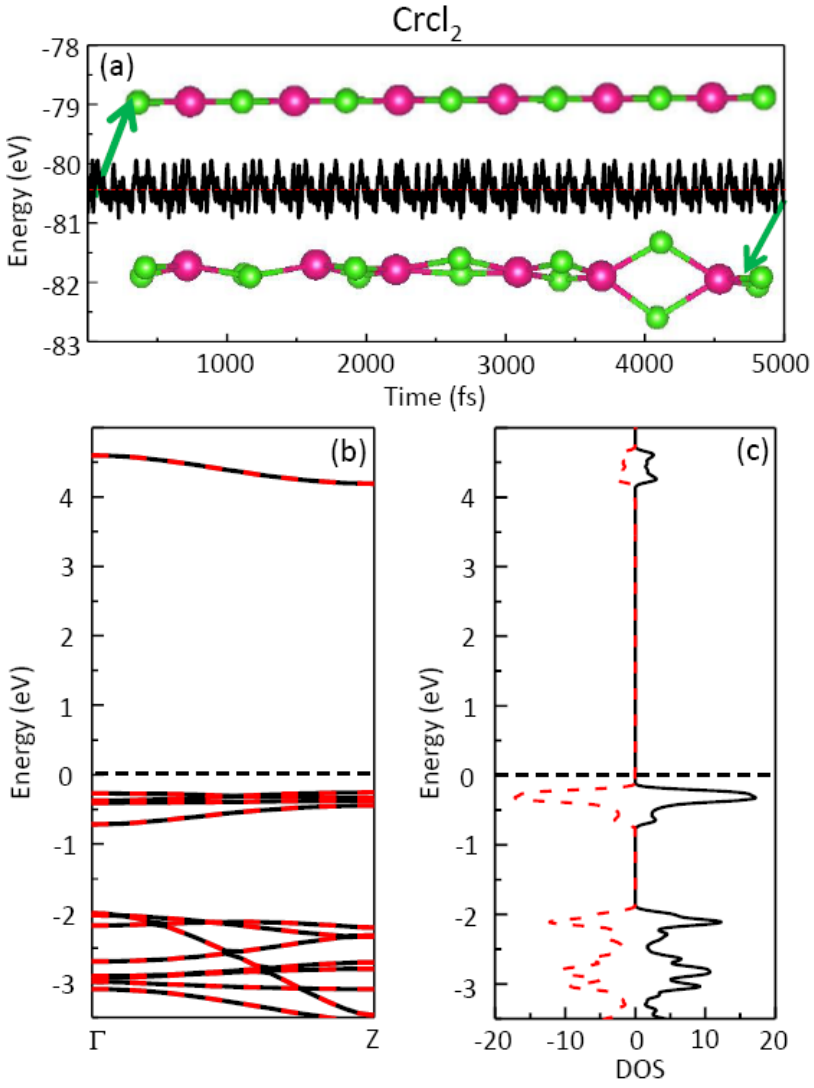

Fig. S1. (a) Evolution of total energy and snapshots of the $CrCl_2$ NW, which is obtained from molecular dynamics (MD) simulations at 5 ps. (b) Energy band structures of the $CrCl_2$ NW, which are calculated at the HSE06 level, and the corresponding spin-resolved DOSs are plotted in the figure (c).

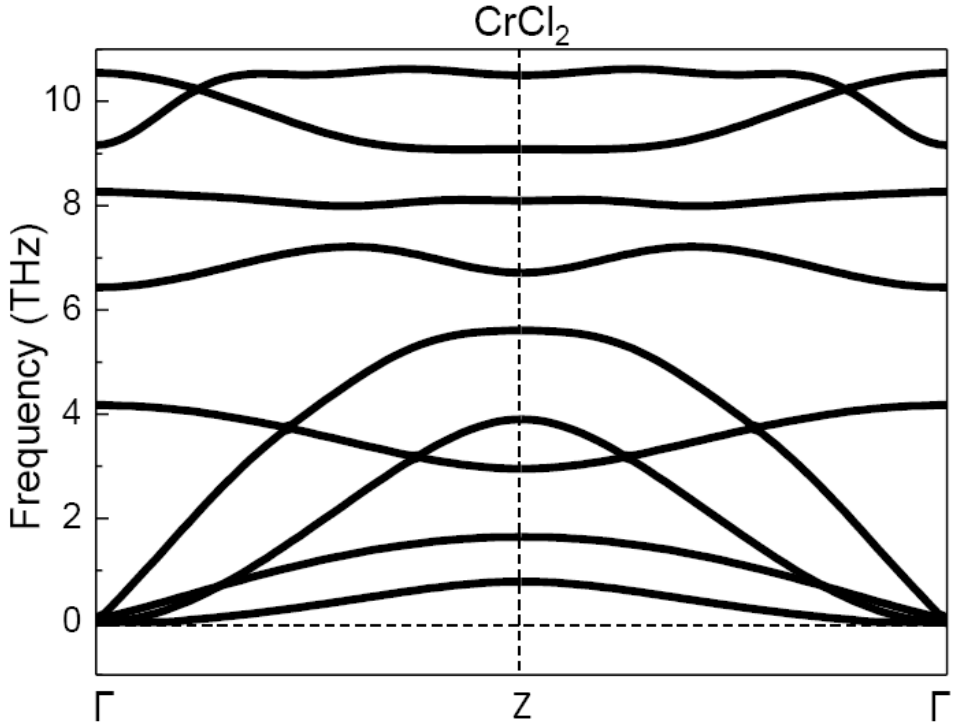

Fig. S2. Phonon dispersion characteristics of the CrCl2 NW, which are calculated by using the PHONOPY package combined with the VASP code.

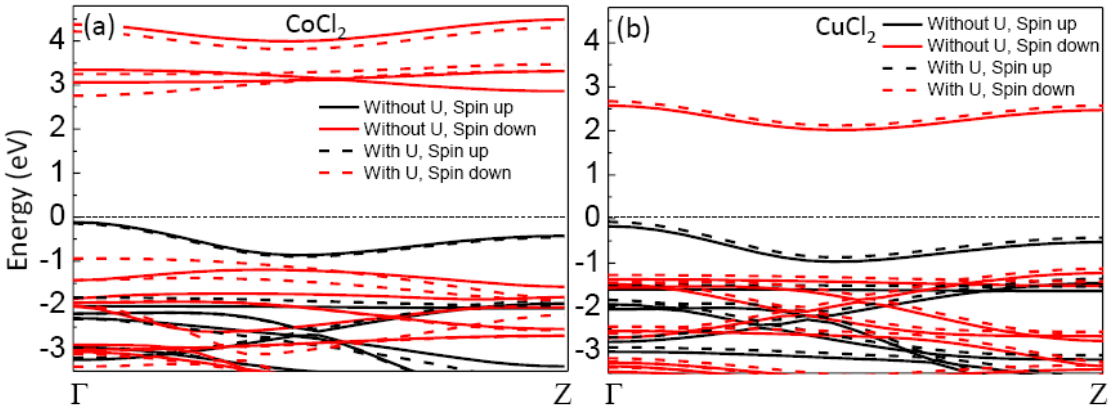

Fig. S3. The spin-dependent band structures of the $CoCl_2$ NW in (a), and those of the $CuCl_2$ NW in (b). The numerical data denoted by the solid lines are calculated by using LDA within the scheme of HSE06 functions, and the numerical data by the solid dash lines are calculated within the scheme of HSE06 functions with the Hubbard U interaction. It is noted that in the calculations, the U value for Cu is set as 5.2 eV, and the U value for the Co atoms is set as 6 eV.