Supplemental Material for

"Robust Half-metallicity in Transition Metal Tribromide Nanowire"

Sheng-shi Li,[a,b] Ya-ping Wang,[c] Shu-jun Hu,[b] Duo Chen,[b] Chang-wen Zhang,*[a] and Shi-shen Yan*[b]

† School of Physics and Technology, University of Jinan, Jinan, Shandong, 250022, P. R. China

‡ School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan, Shandong, 250100, P. R. China

§ Advanced Materials Institute, Qilu University of Technology (Shandong Academy of Science), Jinan, Shandong, 250014, P. R. China

Corresponding Authors:

*E-mail: ss_zhangchw@ujn.edu.cn

*E-mail: shishenyan@sdu.edu.cn

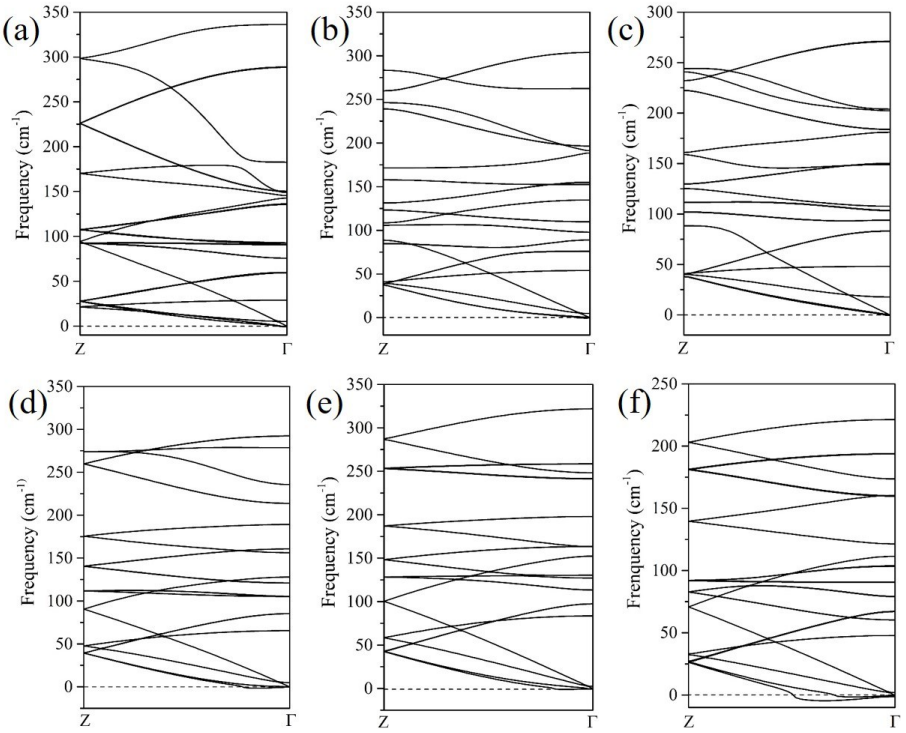

Fig. S1 The calculated phonon spectra of (a) $ScBr_3$, (b) $TiBr_3$, (c) VBr_3, (d) $CrBr_3$, (e) $CoBr_3$, and (f) $CuBr_3$ NWs

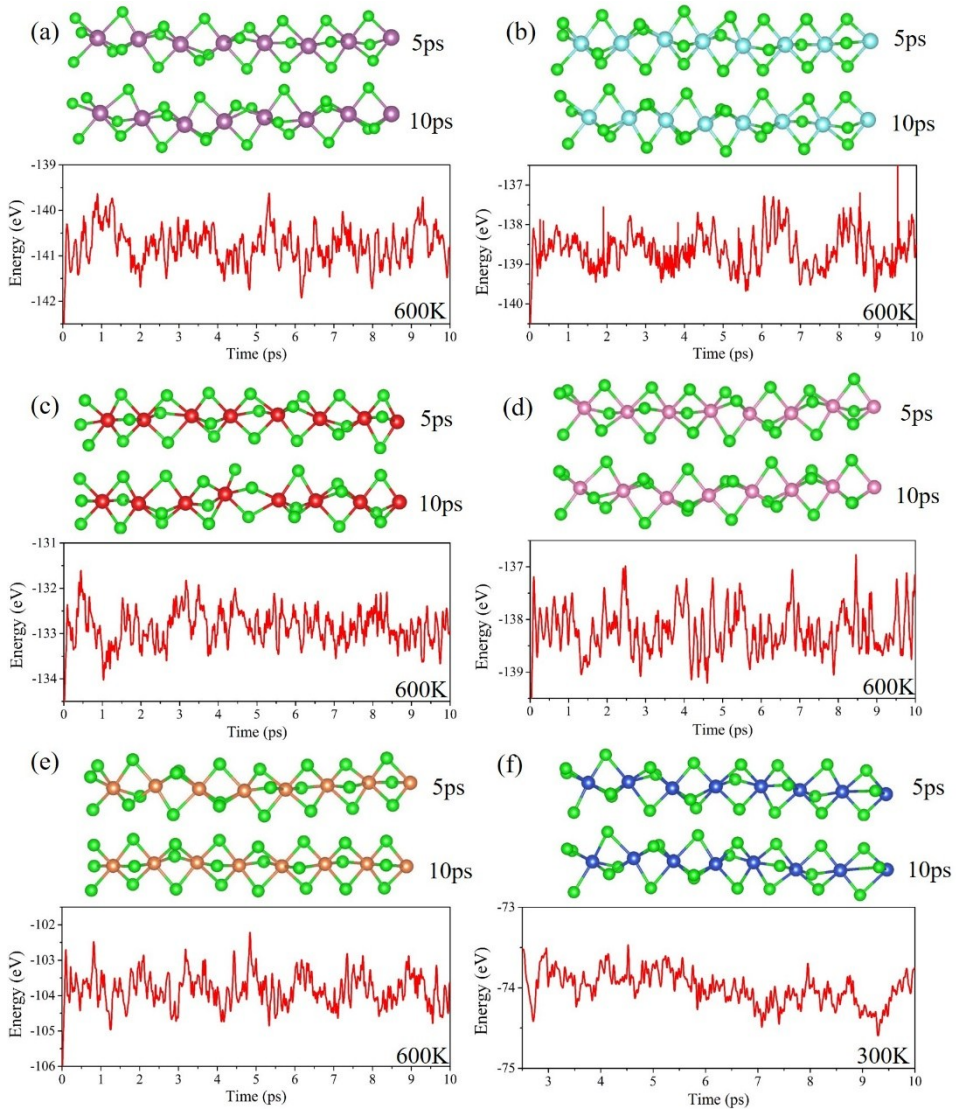

Fig. S2 The snapshot of structure and fluctuation of energy during MD simulation at different temperature for (a) $ScBr_3$, (b) $TiBr_3$, (c) VBr_3, (d) $CrBr_3$, (e) $CoBr_3$, and (f) $CuBr_3$ NWs.

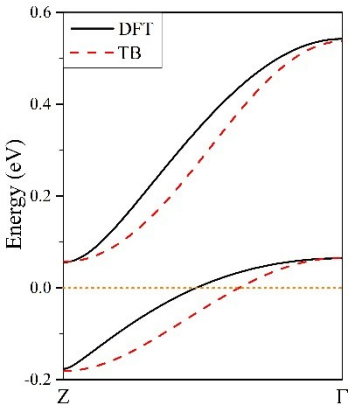

Fig. S3 A comparison of band structure near the Fermi level between DFT and TB results.

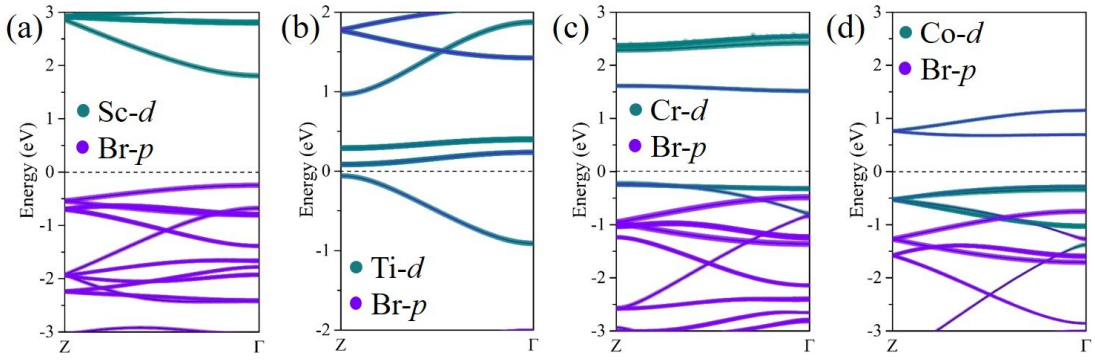

Fig. S4 The calculated band structure of (a) $ScBr_3$, (b) $TiBr_3$, (c) $CrBr_3$, and (d) $CoBr_3$ NWs.

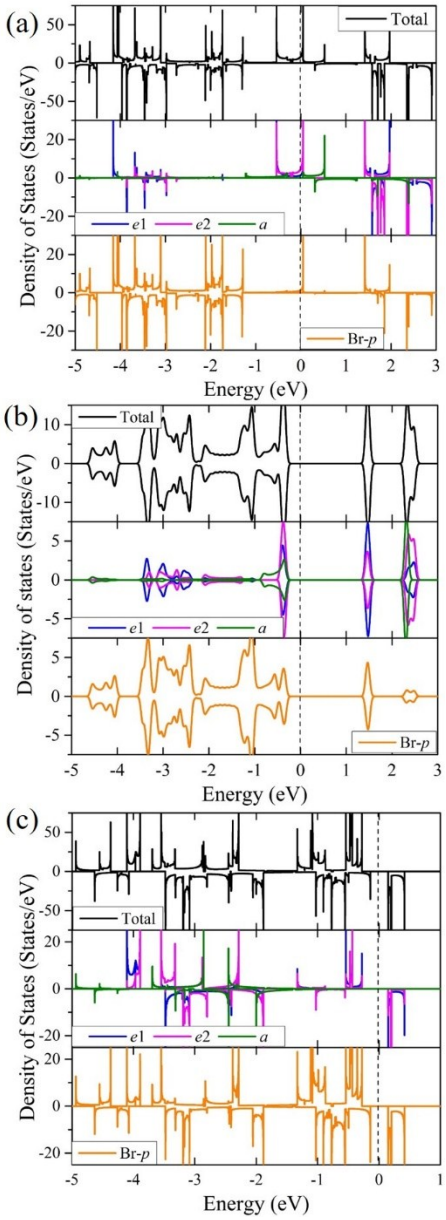

Fig. S5 The plotted TDOS and PDOS of (a) VBr_3, (b) $CrBr_3$, (c) $CuBr_3$ NWs.

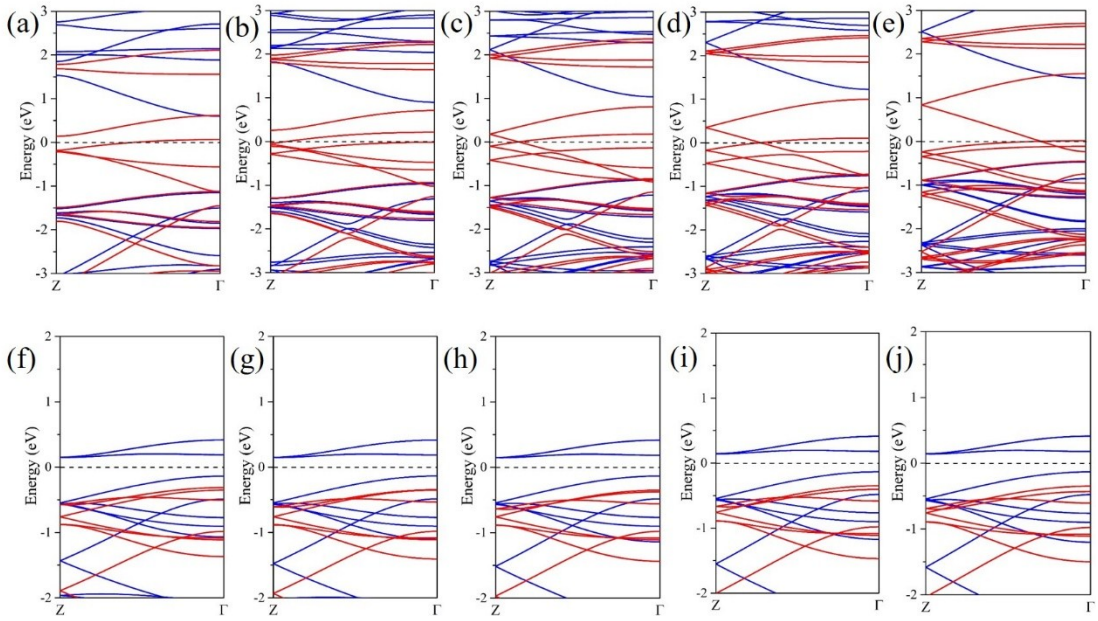

Fig. S6 The band structure evolution of VBr_3 (a-e) and $CuBr_3$ (f-j) NWs under different U value of 0.5, 1.0, 1.5, 2.0, and 2.5eV, respectively. The red and blue line separately represent the spin up and down channels.

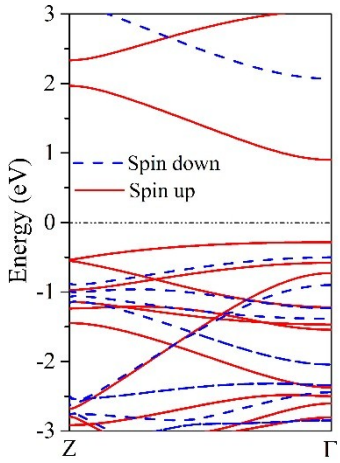

Fig. S7 The calculated band structure of VBr_3 NW with hybrid HSE06 functional.

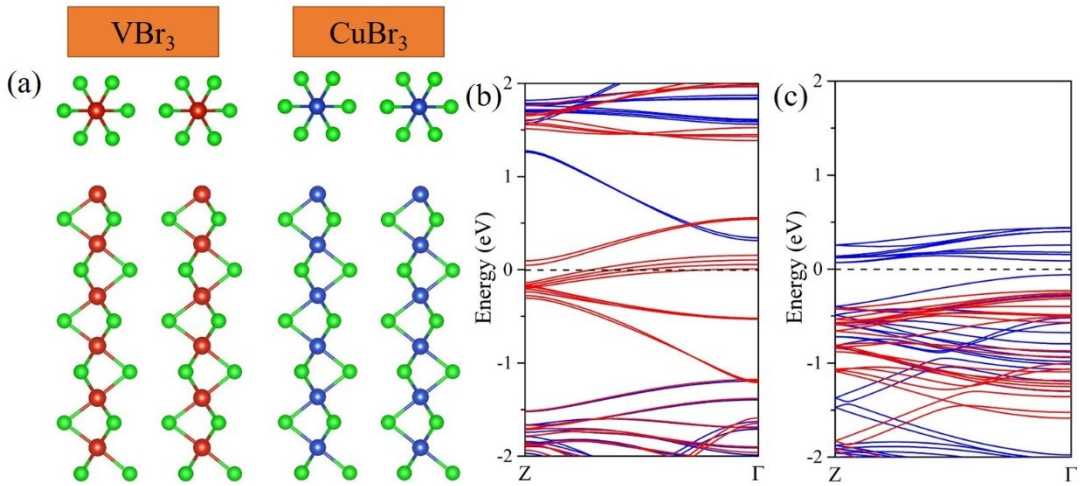

Fig. S8 (a) The bundles composed of VBr_3 and $CuBr_3$ NWs, respectively. (b-c) The calculated spin-resolved band structures. The red and blue lines separately represent the spin up and down channels.