Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Modulation of electronic properties and spin polarization of 2H VS_2 nanoribbons by tuning ribbons widths and edge decoration

Rumeng Zhao[ab], Tianxing Wang[b]*, Mingyu Zhao[c], Congxin Xia[b]*, Yipeng An[b], Xianqi Dai[b]

[a] *School of Physics, Beihang University, Beijing, 100191, China*

[b]*School of Physics and Materials Science, Henan Normal University, Xinxiang, Henan 453600, China*

[c] *School of Physics, Southeast University, Nanjing, 211189, China*

Fig. S1 Four representative magnetic configurations of VS_2: (a) FM, (b) AF-stripy, (c) AF-Neel and (d) AF-zigzag. The positive and negative symbols stand out two opposite spin directions of V atoms along the out-of-plane direction.

Fig. S2 The function of magnetic susceptibility χ_m and phase transition temperature T_C of n =20 zigzag 2H VS_2 nanoribbons with terminated edge of hydrogenated S systems.

Fig. S3 The calculated band structures of zigzag and armchair VS_2 nanoribbons with different edges and widths (n= 4, 5, 6, 7, 8, 10, 13, 15, 20), respectively.

Fig. S4 The spin charge density distributions of zigzag and armchair VS_2 nanoribbons. The isosurface value for all the cases is taken as 0.03 $eÅ^{-3}$. The green (blue) indicates the positive (negative) distribution values.

Table. S1 The edge or sub-edge bonds of zigzag and armchair VS_2 nanoribbons with different terminated edges and widths (n = 4, 5, 6, 7, 8, 10, 13, 15, 20).

Table. S2 Total energies in the FM (E_{FM}) and different AFM states ($E_{AFM\text{-}neel}$, $E_{AFM\text{-}zigzag}$, and $E_{AFM\text{-}stripy}$) of zigzag 2H VS_2 nanoribbons with terminated edge of hydrogenated S systems and different widths (n = 4, 5, 6, 7, 8, 10, 13, 15, 20).

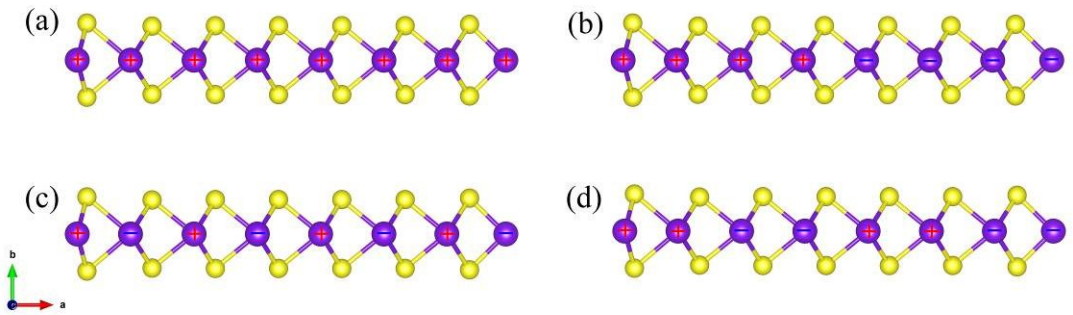

Figure S1. Four representative magnetic configurations of VS_2: (a) FM, (b) AF-stripy, (c) AF-Neel and (d) AF-zigzag. The positive and negative symbols stand out two opposite spin directions of V atoms along the out-of-plane direction.

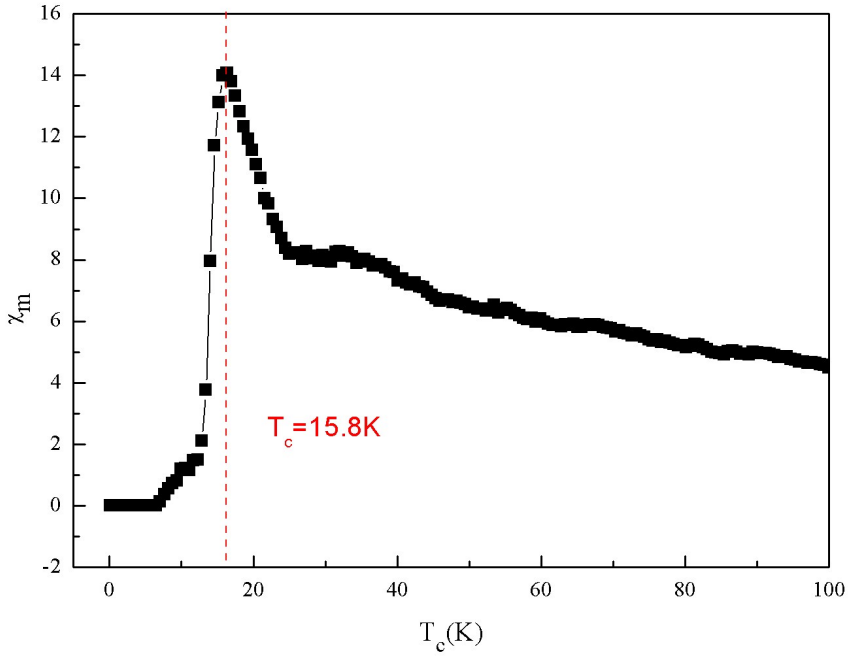

Fig. S2 The function of magnetic susceptibility χ_m and phase transition temperature T_C of n =20 zigzag 2H VS_2 nanoribbons with terminated edge of hydrogenated S systems.

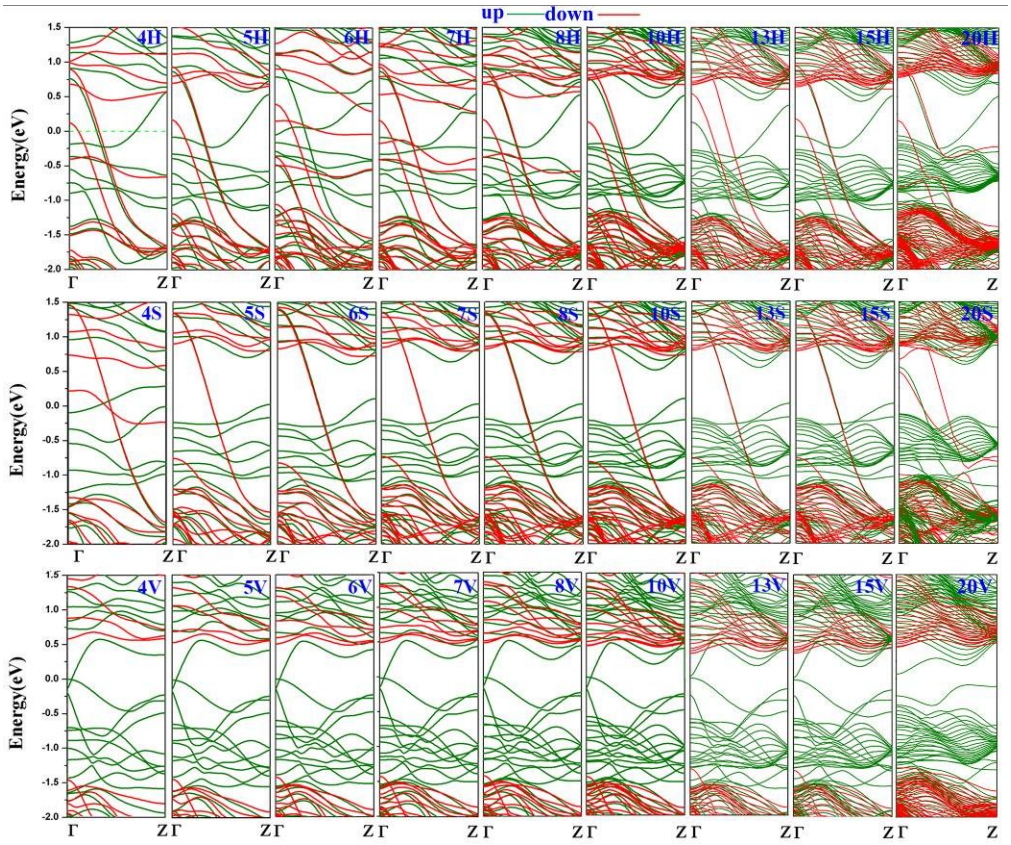

Fig. S3 The calculated band structures of zigzag and armchair VS_2 nanoribbons with different edges and widths (n= 4, 5, 6, 7, 8, 10, 13, 15, 20), respectively.

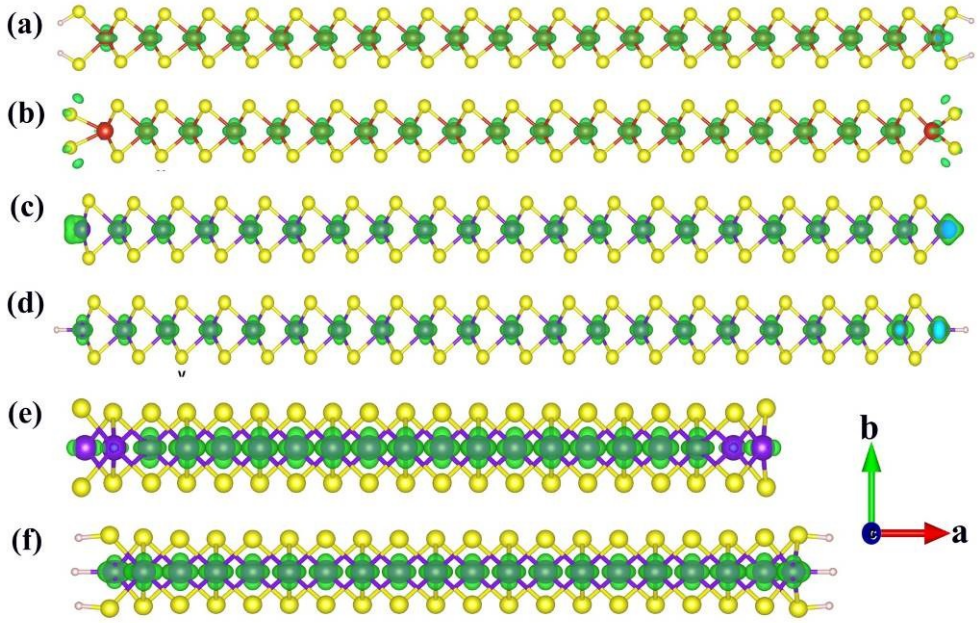

Fig. S4 The spin charge density distributions of zigzag and armchair VS_2 nanoribbons. The isosurface value for all the cases is taken as 0.03 $eÅ^{-3}$. The green (blue) indicates the positive (negative) distribution values.

Types	terminated edge		4	5	6	7	8	10	13	15	20
Zigzag	H_S	edge	2.37	2.38	2.38	2.38	2.38	2.37	2.38	2.38	2.38
		Sub-edge	2.35	2.35	2.36	2.35	2.35	2.36	2.35	2.35	2.35
	S	edge	2.36	2.37	2.37	2.37	2.37	2.38	2.37	2.37	2.37
		Sub-edge	2.33	2.33	2.33	2.33	2.33	2.33	2.33	2.33	2.33
	H_V	edge	2.14	2.15	2.15	2.15	2.15	2.16	2.15	2.15	2.15
		Sub-edge	2.46	2.45	2.44	2.45	2.45	2.44	2.45	2.45	2.45
	V	edge	2.30	2.30	2.30	2.30	2.30	2.30	2.30	2.29	2.30
		Sub-edge	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36	2.36
Armchair	H_(S, V)	Edge1	2.24	2.26	2.25	2.26	2.24	2.25	2.26	2.26	2.26
		Edge2	2.45	2.46	2.54	2.45	2.55	2.55	2.45	2.45	2.45
		Sub-edge	2.39	2.38	2.38	2.40	2.37	2.38	2.38	2.40	2.40
	(S, V)	edge	2.15	2.17	2.28	2.17	2.17	2.17	2.17	2.17	2.17
		Sub-edge	2.36	2.35	2.21	2.35	2.35	2.35	2.35	2.35	2.34
		Sub-edge	2.43	2.40	2.33	2.40	2.40	2.40	2.39	2.39	2.39

Table. S1 The edge or sub-edge bonds of zigzag and armchair VS_2 nanoribbons with different terminated edges and widths (n = 4, 5, 6, 7, 8, 10, 13, 15, 20).

S_H	4	5	6	7	8	10	13	15	20
E_{neel}(eV)	-87.12	-103.63	-120.13	-136.61	-153.11	-186.17	-235.79	-268.75	-.351.53
E_{zigzag}(eV)	-87.23	-103.84	-120.30	-136.95	-153.41	-186.55	-236.30	-269.42	-352.94
E_{stripy}(eV)	-87.23	-103.80	-120.46	-137.08	-153.67	-186.35	-236.72	-269.94	-352.52
E_{FM}(eV)	-88.93	-104.27	-120.90	-137.49	-154.10	-187.34	-236.80	-270.35	-353.09

Table. S2 Total energies in the FM ($E_{FM)}$) and different AFM states ($E_{AFM\text{-}neel}$, $E_{AFM\text{-}zigzag}$, and $E_{AFM\text{-}stripy}$) of zigzag 2H VS_2 nanoribbons with terminated edge of hydrogenated S systems and different widths (n = 4, 5, 6, 7, 8, 10, 13, 15, 20).