Supplementary Materials for "Tunable Magnetic and Electronic Properties of CrS_2/VS_2 Lateral Superlattices"

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Content

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Table S1. Structural parameters of the FM and sAFM states for monolayers 1T-CrS_2 and 2H-VS_2.

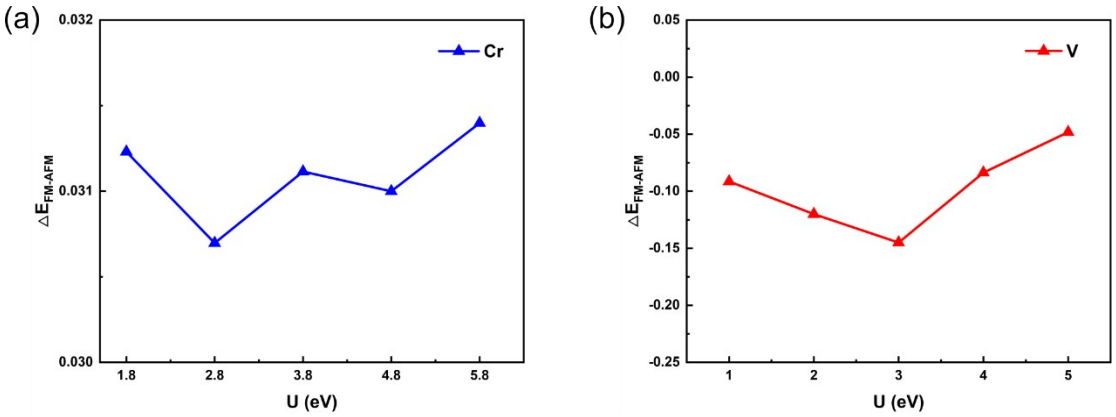

Figure S1. The energy differences between the ferromagnetic and antiferromagnetic states of monolayers (a) 1T-CrS_2 and (b) 2H-VS_2 for different effective U values.

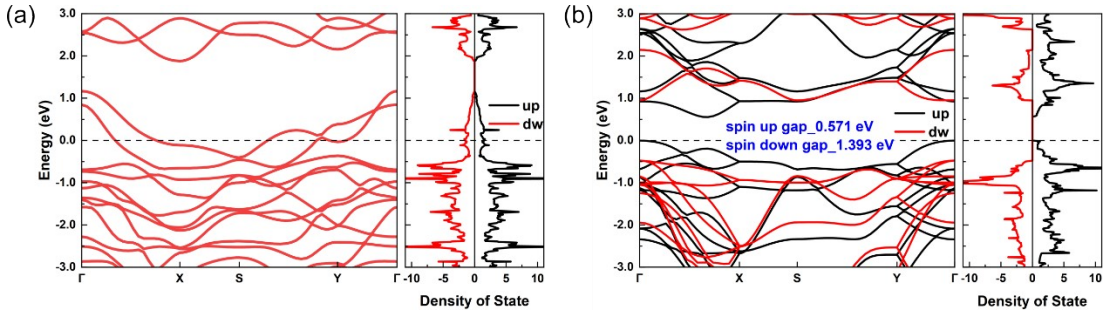

Figure S2. Band structures and density of states of monolayer (a) CrS_2 and (b)VS_2.

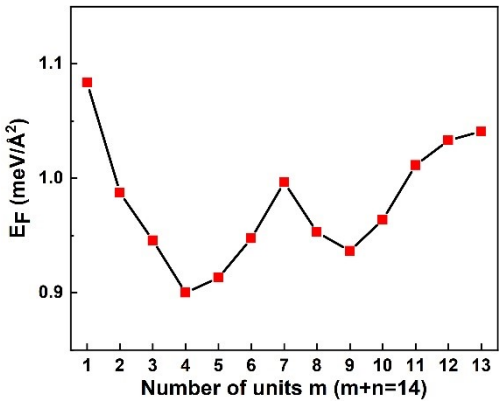

Figure S3. The formation energy of the lateral superlattice $CrS_2(m)/VS_2(n)$ (m+n=14) as a function of the width (m) of the CrS2 sublattice.

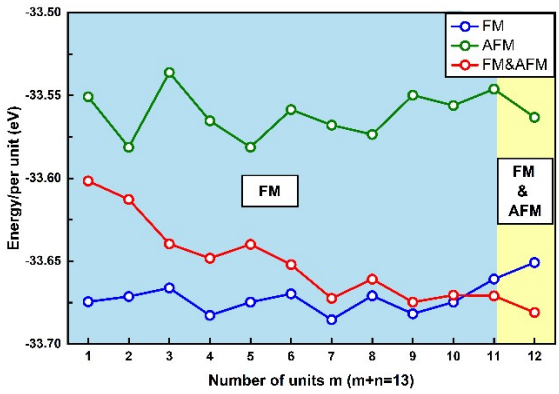

Figure S4. The energy profiles of various magnetic configurations evolve as a function of the number of units for m+n=13.

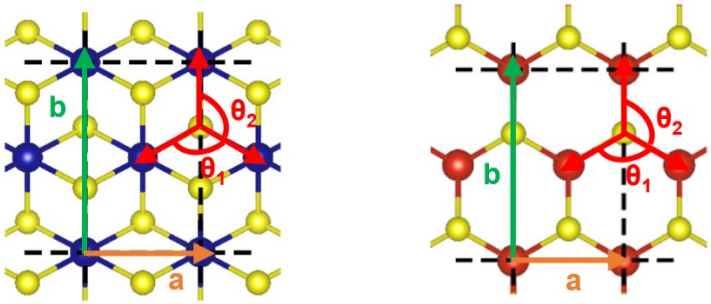

Figure S5. Top view of monolayers (a) 1T-CrS_2 and (b) 2H-VS_2. The orange and green arrows correspond to lattice constants a and b. The red arcs represent the Cr-S-Cr (V-S-V) angles θ_1 and θ_2, respectively.

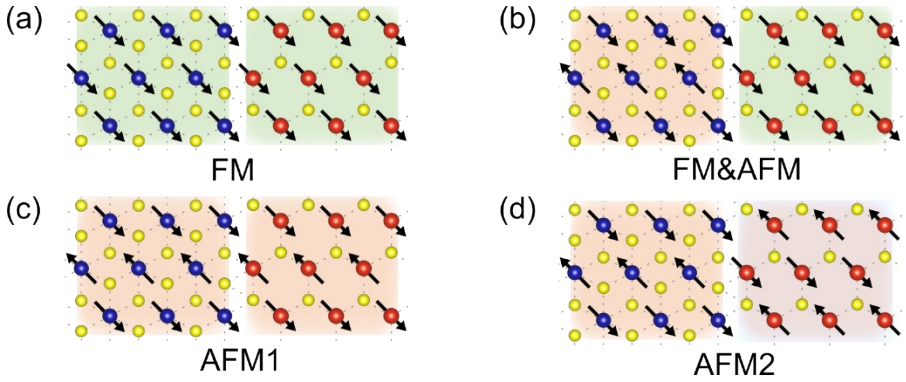

Figure S6. Schematic diagrams illustrating three magnetic orders used for the calculation of exchange parameters: (a) FM, (b) FM&AFM, (c) AFM1 and (d) AFM2.

Spin-exchange coupling parameters (see Fig. 4(a)) were extracted by calculating the total energy differences of eight magnetic configurations (see Fig. S4(a)-(d)) based on the Heisenberg model. The energy contributed by magnetic interaction in these magnetic orders in a unit cell is expressed as

$$E_1 = -2\times(m-1)\times S_{Cr}^2\times 3J_1 - 2\times(n-1)\times S_V^2\times 3J_2 - 2\times S_{Cr}S_V\times 3J_3 + H_0$$

$$E_2 = 2\times(m-1)\times S_{Cr}^2\times J_1 - 2\times(n-1)\times S_V^2\times 3J_2 + 2\times S_{Cr}S_V\times 3J_3 + H_0$$

$$E_3 = 2\times(m-1)\times S_{Cr}^2\times J_1 + 2\times(n-1)\times S_V^2\times J_2 + 2\times S_{Cr}S_V\times 3J_3 + H_0$$

$$E_4 = 2\times(m-1)\times S_{Cr}^2\times J_1 + 2\times(n-1)\times S_V^2\times J_2 - 2\times S_{Cr}S_V\times 3J_3 + H_0 \quad \text{(S1)}$$

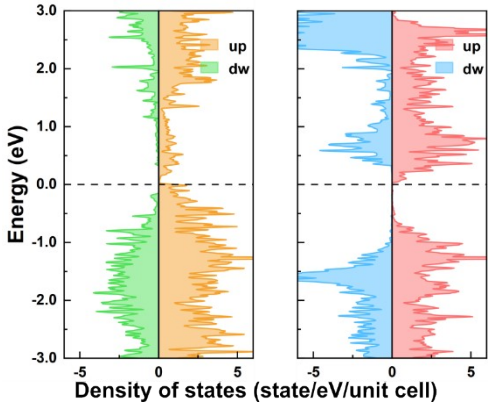

Figure S7. Projected density of states of the central unit cells of CrS_2 and VS_2 in the $CrS_2(7)/VS_2(7)$ superlattice.

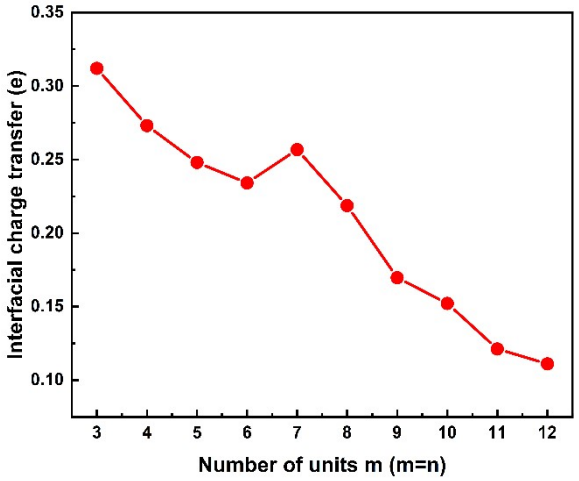

Figure S8. The charge transfer at the interface from the CrS_2 ribbon to the VS_2 ribbon as a function of the number of units for m=n.

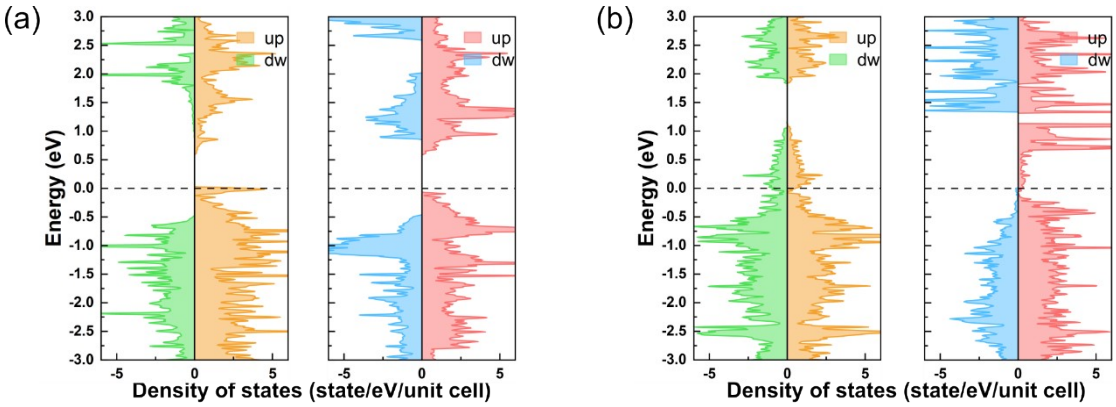

Figure S9. Projected density of states of the central unit cells of CrS_2 and VS_2 in the (a) $CrS_2(1)/VS_2(13)$ and (b) $CrS_2(13)/VS_2(1)$ superlattices.

Table S1. Structural parameters of the FM and sAFM states for monolayers 1T-CrS_2 and 2H-VS_2.

	a (Å)	b (Å)	θ_1 (°)	θ_2 (°)
CrS_2-sAFM	3.34	5.51	88.58	84.85
CrS_2-FM	3.33	5.76	88.61	88.21
VS_2-sAFM	3.22	5.64	86.42	86.20
VS_2-FM	3.22	5.57	87.66	87.62