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Supplemental materials for "Strain-induced magnetic phase transition, magnetic anisotropy switching and bilayer antiferromagnetic skyrmions in van der Waals magnet $CrTe_2$"†

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1 Critical temperature of $CrTe_2$ monolayer under strain.

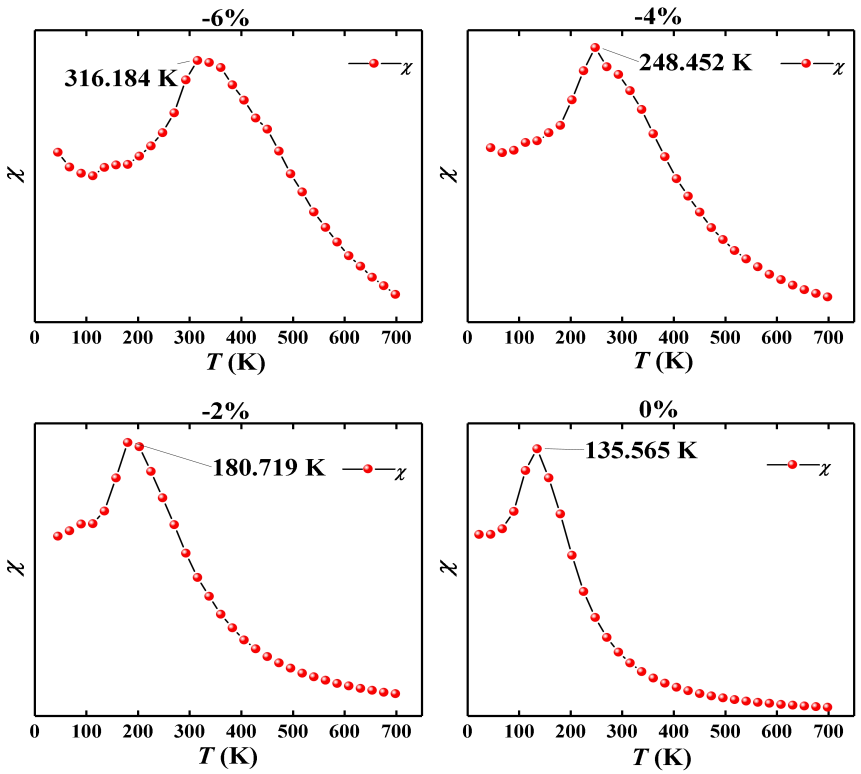

Fig. S1 The critical temperature (T_c) of $CrTe_2$ monolayer without strain and with compressive strain.

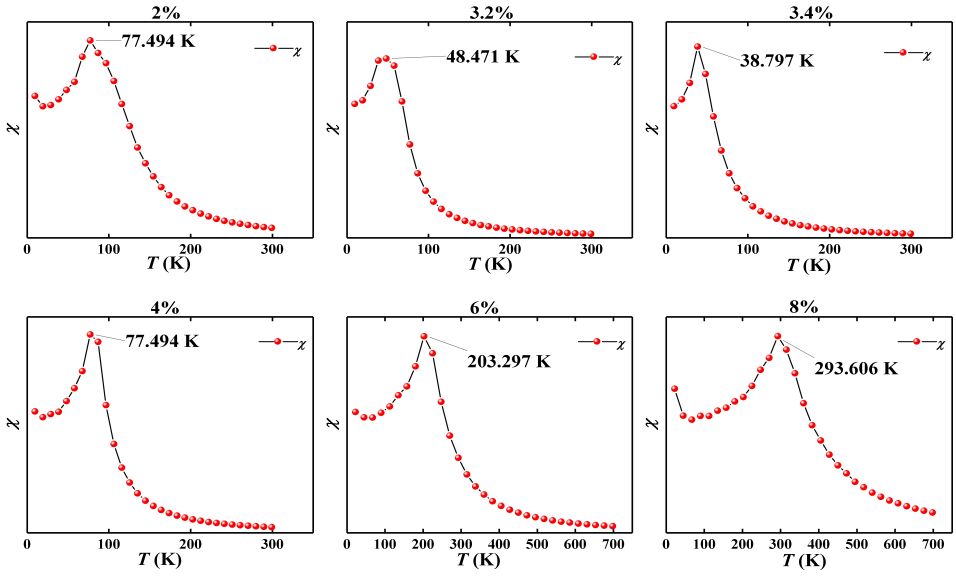

Fig. S2 The critical temperature (T_c) of $CrTe_2$ monolayer with tensile strain.

Table S1 Optimized lattice parameters a, Heisenberg exchange coefficients J_1, J_2, J_3, single-ion anisotropy K and the magnetic moments of Cr atoms in $CrTe_2$ monolayer with different biaxial strains.

Strain (%)	a (Å)	J_1 (meV)	J_2 (meV)	J_3 (meV)	K (meV)	M_{Cr} (μ_B)
−6	3.40	38.41	-8.00	11.43	-2.14	2.95
−4	3.47	27.76	-6.68	8.30	-2.91	2.94
−2	3.55	18.96	-5.43	6.28	-2.98	2.97
0	3.62	10.48	-4.56	4.25	-2.12	3.00
2	3.69	2.99	-3.94	2.66	-1.34	3.04
4	3.76	-3.52	-3.46	1.55	-0.97	3.07
6	3.84	-11.07	-3.65	0.78	0.17	3.09
8	3.91	-19.14	-3.01	1.04	3.84	3.14

2 The Heisenberg exchange and Dzyaloshinskii-Moriya interactions in bilayer $CrTe_2$

According to Eq (S1) in the main text, the Heisenberg exchange interactions can be quantitatively estimated by calculating each total energy expression for various spin configurations as expressed below.

$$E_1 = (36J_1 + 36J_2 + 36J_3 + 6J_{z1} - 4J_{z2} - 12J_{z3})S^2 + E_0, \tag{S1}$$

$$E_2 = (-4J_1 - 12J_2 + 4J_3 + 6J_{z1} - 4J_{z2} - 12J_{z3})S^2 + E_0, \tag{S2}$$

$$E_3 = (4J_1 - 12J_2 + 4J_3 + 2J_{z1} - 4J_{z2} - 12J_{z3})S^2 + E_0, \tag{S3}$$

$$E_4 = (-4J_1 - 12J_2 + 4J_3 + 2J_{z1} + 0J_{z2} - 8J_{z3})S^2 + E_0, \tag{S4}$$

$$E_5 = (-4J_1 - 12J_2 + 4J_3 + 2J_{z1} + 4J_{z2} - 12J_{z3})S^2 + E_0, \tag{S5}$$

$$E_6 = (0J_1 - 12J_2 + 4J_3 + 4J_{z1} + 0J_{z2} - 12J_{z3})S^2 + E_0, \tag{S6}$$

$$E_7 = (0J_1 - 4J_2 + 4J_3 + 2J_{z1} - 4J_{z2} - 12J_{z3})S^2 + E_0. \tag{S7}$$

Here, J_1, J_2, J_3 are the Heisenberg exchange coefficients of first, second and third nearest neighbor of Cr atoms in the same layer, J_{z1}, J_{z2}, J_{z3} are the Heisenberg exchange coefficients of first, second and third nearest neighbor of Cr atoms in different layers, K is the single-ion anisotropy and E_0 is the non-magnetic section of the total energy. The calculated magnetic parameters are listed in Tab. S2

We choose the four states energy mapping method to calculate the Dzyaloshinskii-Moriya interaction (DMI) in bilayer $CrTe_2$. Take the x component of DMI (d_x) as an example. We choose a pair of the nearest Cr atoms labeled $\vec{S}_1$ and $\vec{S}_2$ to set the four spin configurations as shown in Tab. S3. Notice that the spins of all the other spin sites are the same and are along the Z direction. Then, d_x can be obtained by:

$$d_x = \frac{E_1 + E_4 - E_2 - E_3}{4S^2}. \tag{S8}$$

The calculated d_x, d_y and d_z are listed in Tab. S2

Table S2 Heisenberg exchange coefficients and DMI of bilayer $CrTe_2$.

J_1(meV)	J_2(meV)	J_3(meV)	J_{z1}(meV)	J_{z2}(meV)	J_{z3}(meV)	d_x(meV)	d_y(meV)	d_z(meV)
-1.69	-0.70	-2.54	1.25	0.78	0.44	0.54	0.56	1.33

Table S3 Spin configurations used to calculate d_x, d_y and d_z.

DMI	d_x(meV)		d_y(meV)		d_z(meV)	
States	S1	S2	S1	S2	S1	S2
1	(0,S,0)	(0,0,S)	(0,0,S)	(S,0,0)	(S,0,0)	(0,S,0)
2	(0,S,0)	(0,0,-S)	(0,0,S)	(-S,0,0)	(S,0,0)	(0,-S,0)
3	(0,-S,0)	(0,0,S)	(0,0,-S)	(S,0,0)	(-S,0,0)	(0,S,0)
4	(0,-S,0)	(0,0,-S)	(0,0,-S)	(-S,0,0)	(-S,0,0)	(0,-S,0)