Supporting Information

$CrSbS_3$ monolayer: a potential phase transition ferromagnetic semiconductor

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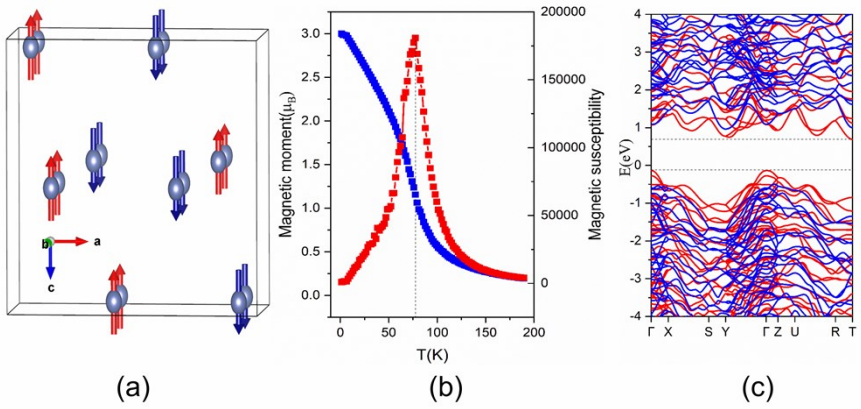

Fig. S1 (a) Schematics of antiferromagnetic ground state for bulk $CrSbS_3$ when the value of U is greater than 3 eV. The nonmagnetic atoms are omitted. (b) Evolution of spin magnetic moment per formula (blue line) and magnetic susceptibility (red line) with respect to temperature for bulk $CrSbS_3$. (c) Band structure of bulk $CrSbS_3$ with PBE+U functional.

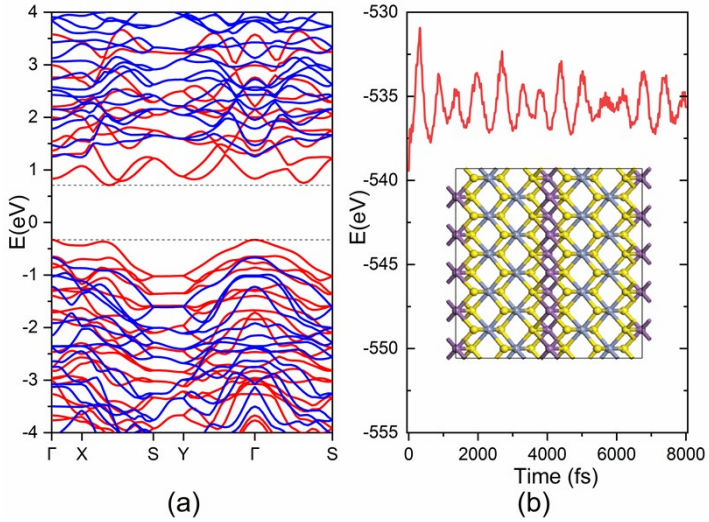

Fig. S2 (a) Band structure of $CrSbS_3$ monolayer with PBE+U functional. (b) AIMD evolution of energy for $CrSbS_3$ monolayer. The inset shows the snapshots of structure at 300 K after 8 ps AIMD simulation.

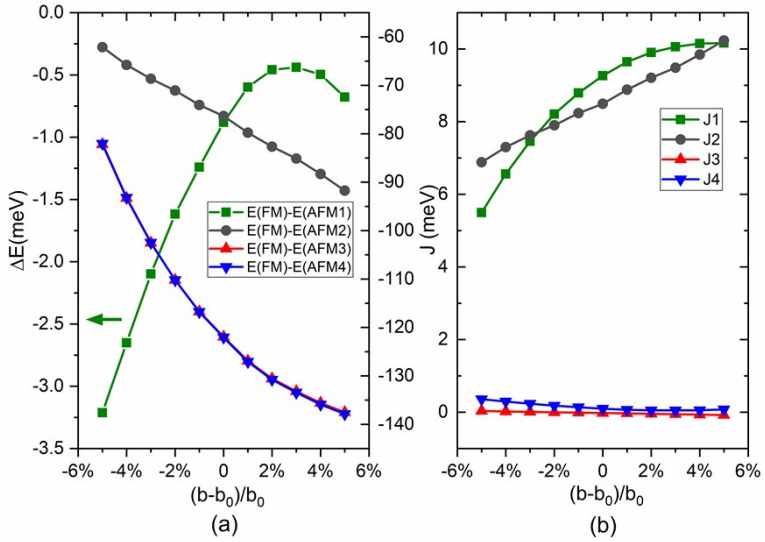

Fig. S3 (a) Relative energies of AFM1 (green line), AFM2 (black line), AFM3 (red line) and AFM4 states (blue line) compared to FM state when applying uniaxial strain along b axis. The left longitudinal axis corresponds to the energy difference between FM and AFM1, while others correspond to the right longitudinal axis. (b) The variation of four exchange parameters $J_1(green\ line)$,$J_2(black\ line)$ $J_3(red\ line)$, $J_4(blue\ line)$ with the strain along b axis.

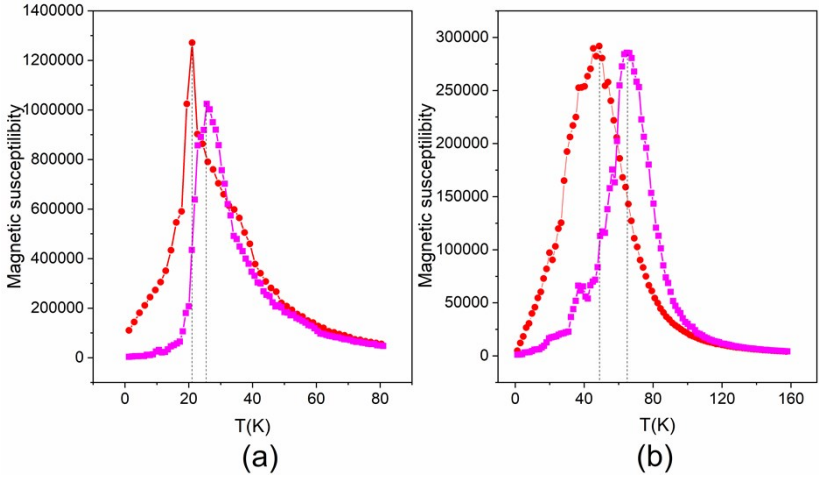

Fig. S4 The simulated magnetic susceptibility curves with (purple line) and without (red line) considering magnetic anisotropy for (a) pristine $CrSbS_3$ monolayer and (b) 5% compressed system with strain parallel to the CrS_6 chain.

Table S1. When applying uniaxial strain χ perpendicular or parallel to the CrS_6 chain, the calculated band gap and spin exchange splitting gaps for FM state $CrSbS_3$ monolayer. Results are based on PBE+U functional.

The formula of χ	χ (%)	Band gap (eV)	Δ_1 (eV)	Δ_2 (eV)
$(a-a_0)/a_0$	-1	1.019	0.5310	0.3508
	0	1.039	0.5305	0.3369
	1	1.056	0.5234	0.3255
	2	1.076	0.4971	0.3140
	3	1.078	0.4941	0.3045
	4	1.074	0.4977	0.2973
	5	1.070	0.4939	0.2950
$(b-b_0)/b_0$	-5	1.102	0.4429	0.2915
	-4	1.099	0.4858	0.3694
	-3	1.093	0.5135	0.3507
	-2	1.084	0.5375	0.3524
	-1	1.061	0.5490	0.3318
	1	1.039	0.4591	0.3454
	1	0.993	0.3959	0.3524
	1	0.971	0.3335	0.3616
	1	0.930	0.2948	0.3724
	1	0.883	0.2642	0.3842

Table S2. The axial anisotropy strength D and planar anisotropy strength E for pristine $CrSbS_3$ monolayer and 5% compressed system with strain parallel to the CrS_6 chain calculated by PBE+U+SOC method.

	Pristine	5% compressed
E(1 0 0) (eV)	-27.05850	-26.95668
E(0 1 0) (eV)	-27.05844	-26.95664
E(0 0 1) (eV)	-27.05847	-26.95428
D (meV)	0.00077	1.05582
E (meV)	-0.01522	-0.00756
T_c (K)	25.2	65.1