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

Room-temperature Ferromagnetism, Half-metallicity and Spin Transport in Monolayer $CrSc_2Te_4$-Based Magnetic Tunnel Junction Devices

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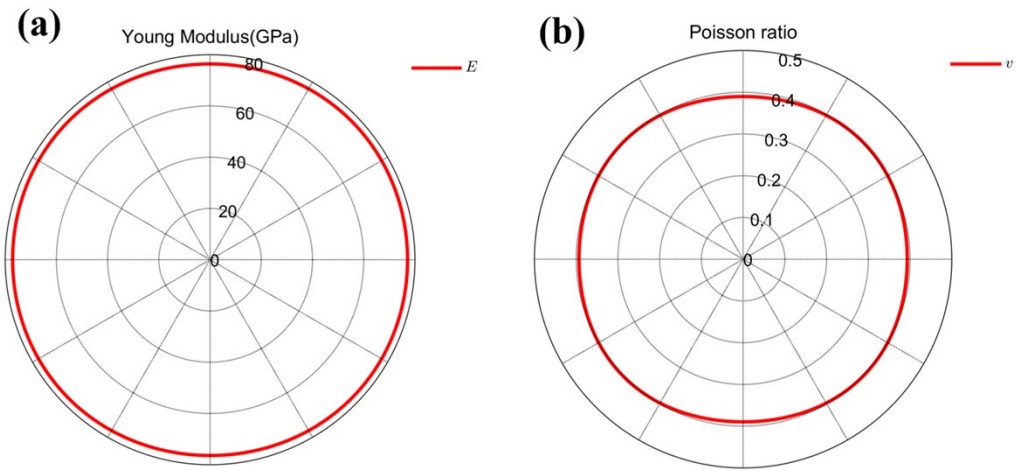

Fig. S1 Calculated orientation-dependent Young's modulus $Y(\theta)$ and Poisson's ratio $v(\theta)$ for $CrSc_2Te_4$ monolayer, respectively.

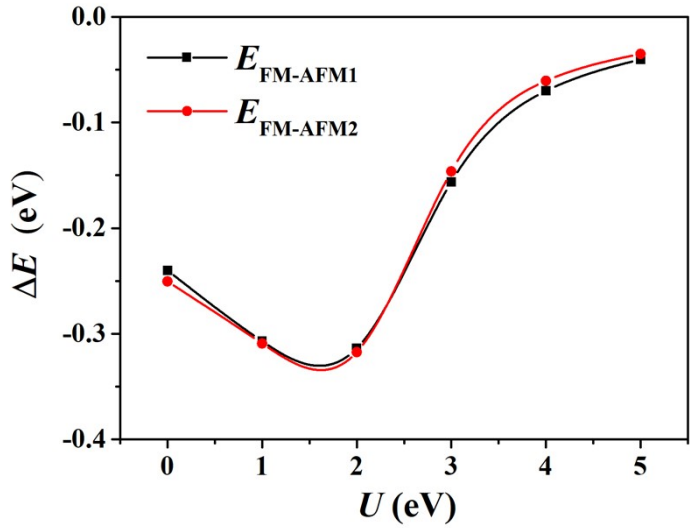

Fig. S2 The calculated energy differences between FM and AFM states for $CrSc_2Te_4$ monolayer with different U values using the PBE method.

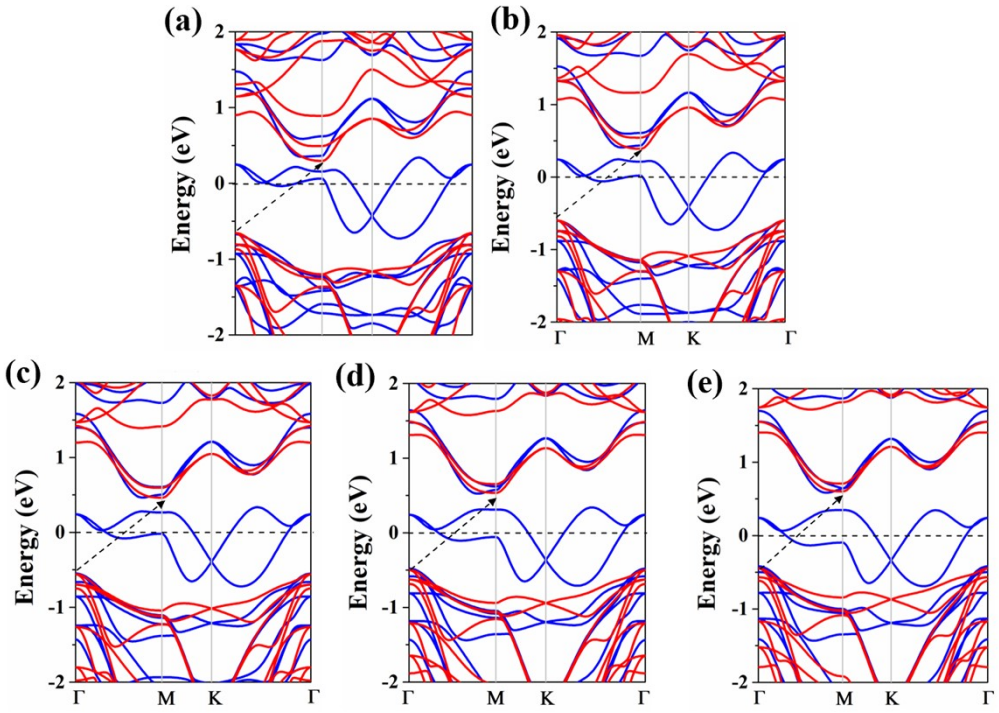

Fig. S3 The calculated band structures of $CrSc_2Te_4$ monolayer with different *U* values using the PBE method. The blue and red lines indicate the spin-up and spin-down, respectively. The Fermi level is set to be 0 eV.

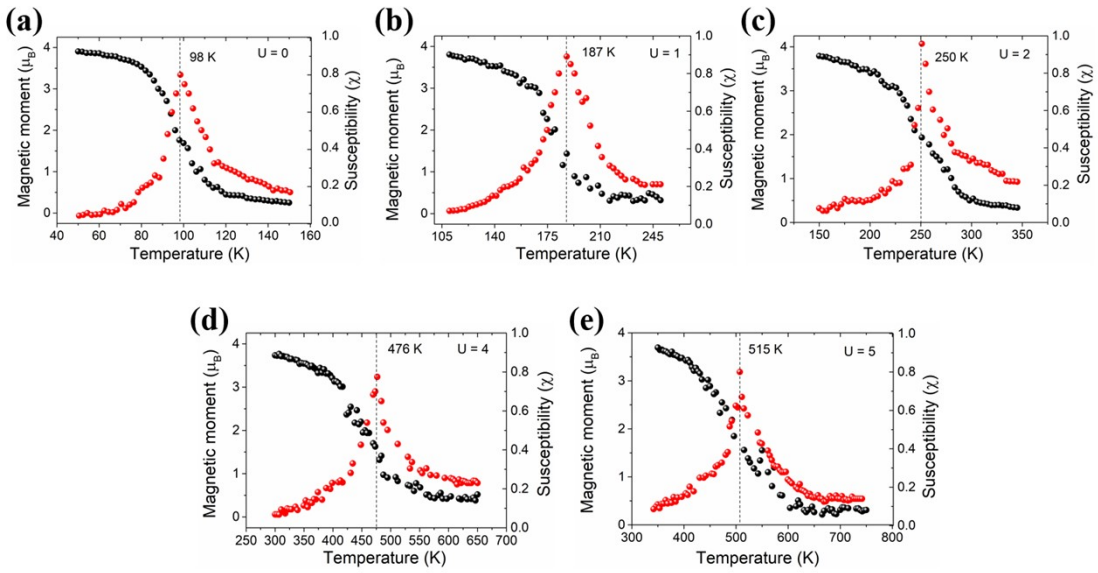

Fig. S4 Dependence of magnetic moment and magnetic susceptibility on the temperature by the Heisenberg model *via* Monto Carlo (MC) simulation of $CrSc_2Te_4$ monolayer with different *U* values.

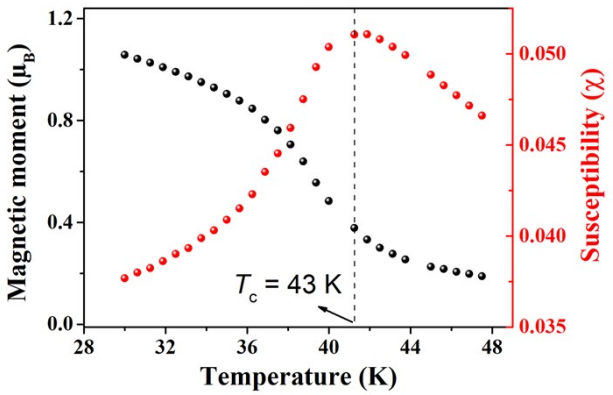

Fig. S5 Dependence of magnetic moment and magnetic susceptibility on the temperature by the Heisenberg model *via* Monto Carlo (MC) simulation of CrI_3 monolayer.

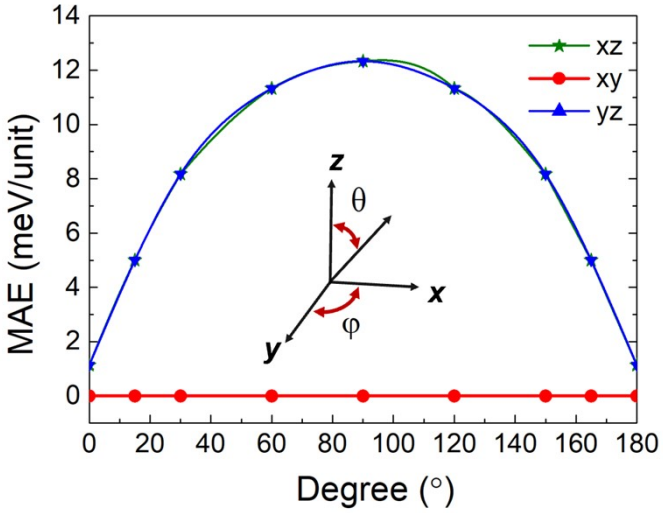

Fig. S6 The variation of magnetic anisotropy energy (MAE) of $CrSc_2Te_4$ monolayer. Among the MAE along the *xy* plane with respect to the polar angle φ, and along the *xz* and *yz* planes with respect to polar angle θ.

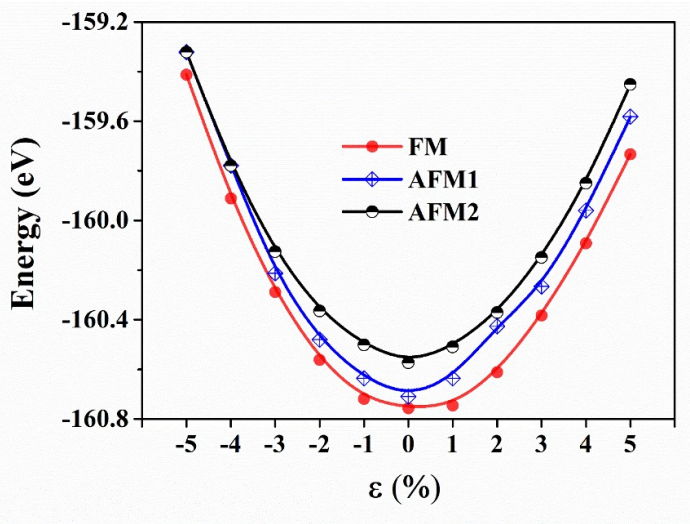

Fig. S7 The energies of different magnetic configurations as a function of strain range from −5% to 5%.

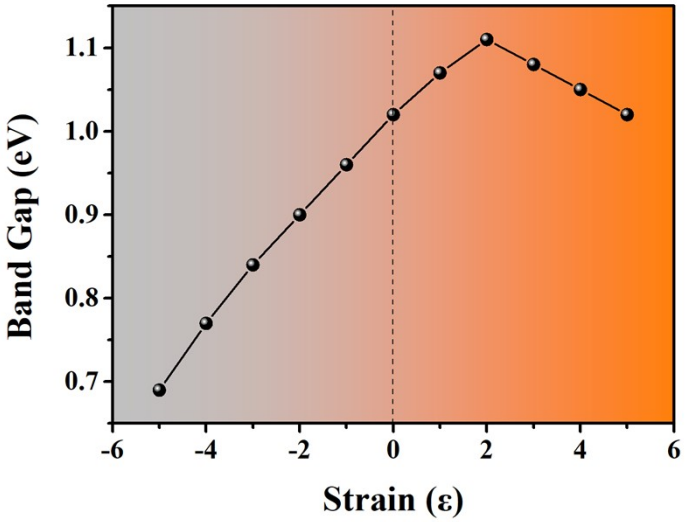

Fig. S8 The variation of band gap of $CrSc_2Te_4$ monolayer under strains (ε) from −5% to 5% using the PBE+U method (U = 3.0 eV).

Table S1 The energy of three magnetic configurations with different U values using the PBE method.

U	0	1	2	3	4	5
FM	-167.776	-165.516	-163.456	-161.585	-159.962	-158.563
AFM1	-167.531	-165.209	-163.143	-161.428	-159.892	-158.522
AFM2	-167.526	-165.207	-163.139	-161.438	-159.902	-158.528

Table S2 Magnetic anisotropy energy (MAE, meV/Cr atom) per Cr atom between (100), (010) and (001) direction calculated for $CrSc_2Te_4$ monolayer by PBE+*U* (*U* from 0 to 5 eV) method.

$CrSc_2Te_4$	***E* (100)-*E* (001)**	***E* (010)- *E* (001)**	***E* (010)-*E* (100)**
0	-0.428	-0.428	-0.002
1	-0.792	-0.794	-0.001
2	-1.342	-1.351	-0.003
3	-2.451	-2.458	-0.007
4	-1.206	-1.201	-0.001
5	-1.490	-1.493	-0.003