Electronic Supplementary Material (ESI) for RSC Advances.

Intrinsic half-metallicity in two-dimensional Cr_2TeX_2 (X = I, Br, Cl) monolayers

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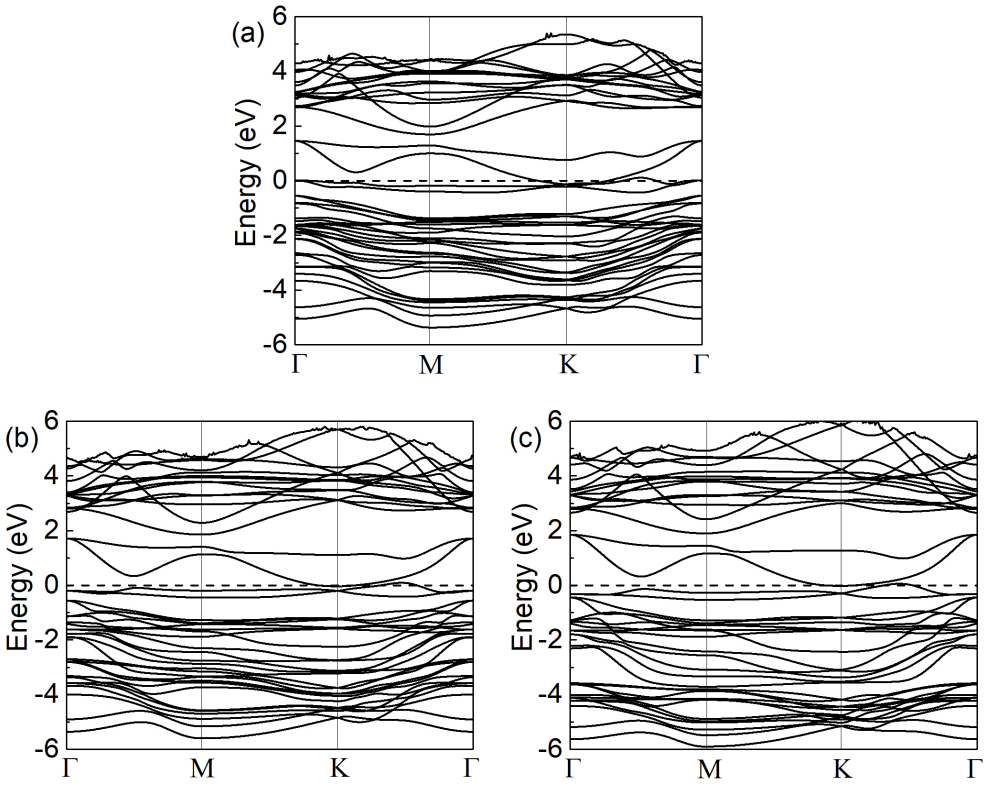

Figure S1. When the SOC is considered, the calculated band structures of Cr_2TeX_2 monolayers: (a) for Cr_2TeI_2, (b) for Cr_2TeBr_2, and (c) for Cr_2TeCl_2. The dashed-black line at zero eV denotes the Fermi energy E_f. The coordinates of the high symmetry points are Γ = (0, 0, 0), M = (0.5, 0, 0), and K = (1/3, 1/3, 0).

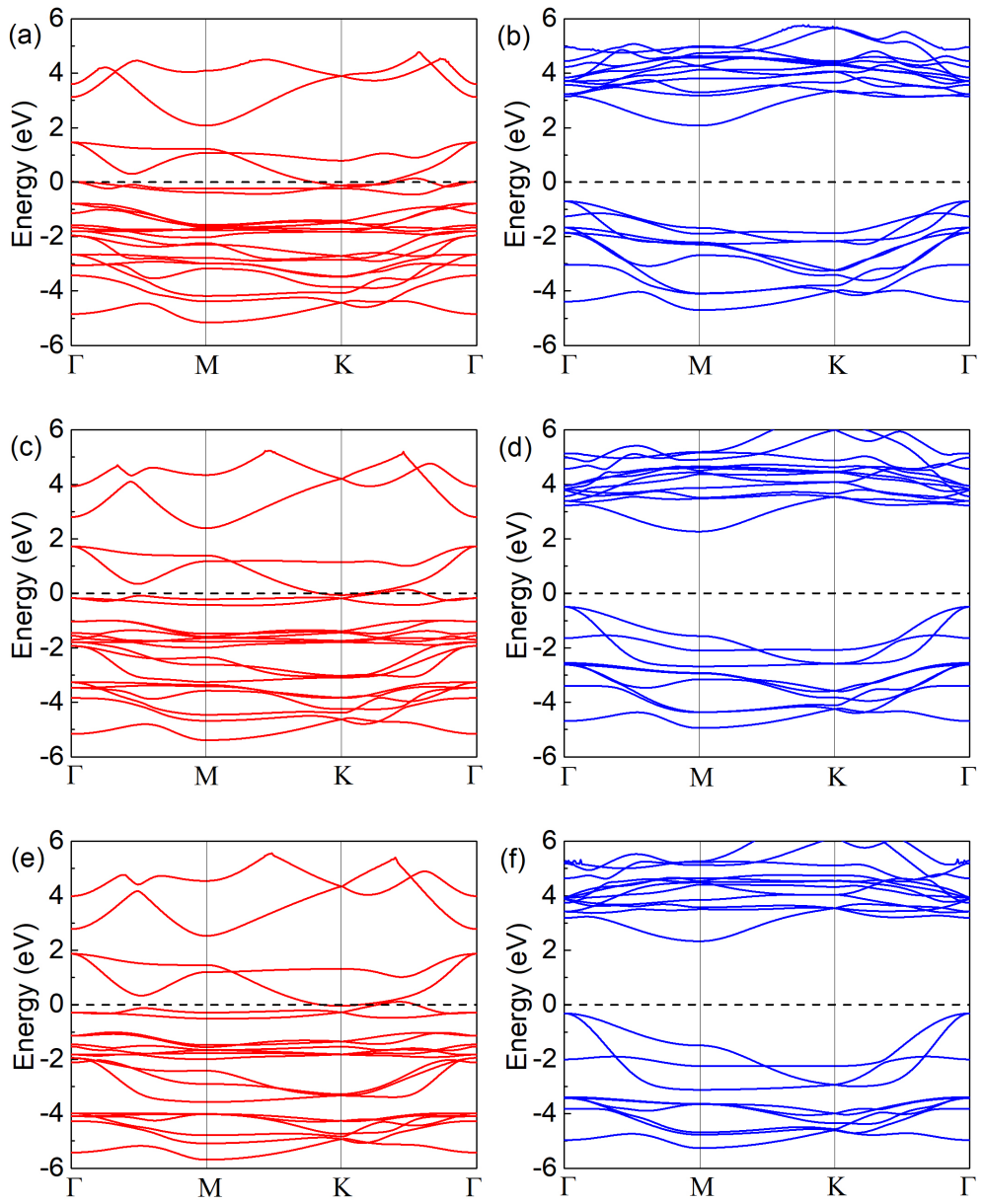

Figure S2. (Color online) When U_{eff} = 3.0 eV, the calculated band structures of Cr_2TeX_2 monolayers with spin-up (left: marked in red color) and spin-down (right: marked in blue color) channels: (a) and (b) for Cr_2TeI_2, (c) and (d) for Cr_2TeBr_2, (e) and (f) for Cr_2TeCl_2. The dashed-black line at zero eV denotes the Fermi energy E_f. The coordinates of the high symmetry points are Γ = (0, 0, 0), M = (0.5, 0, 0), and K = (1/3, 1/3, 0).

Table S1. When the spin-orbit coupling is considered, relative energies of the different magnetic configurations per 2×2×1 supercell. The energy of FM state is taken as zero. J_1 and J_2 represent the intra-sublayer and inter-sublayer exchange parameters, respectively.

	FM *meV*	AFM1 *meV*	AFM2 *meV*	J_1 *meV*	J_2 *meV*
Cr_2TeI_2	0.0	1916.4	1914.8	9.969	19.963
Cr_2TeBr_2	0.0	2428.2	1679.4	6.797	25.294
Cr_2TeCl_2	0.0	2454.7	1710.1	6.967	25.570

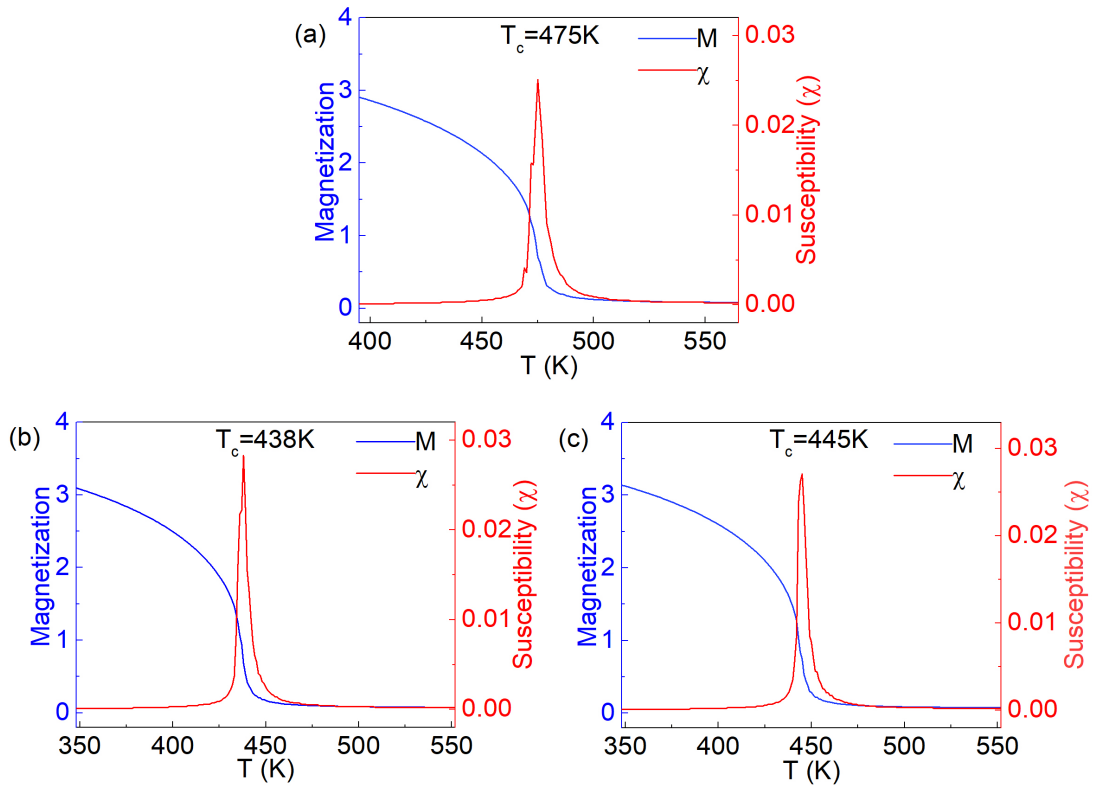

Figure S3. (Color online) When the spin-orbit coupling is considered, the average magnetic moment and susceptibility of the primitive Cr_2TeX_2 monolayer as a function of temperature, obtained from the Monte Carlo simulations with the 2D Heisenberg model: (a) Cr_2TeI_2, (b) Cr_2TeBr_2, and (c) Cr_2TeCl_2. In the MC simulations, the D_i in the Hamiltonian H is taken the positive value for the Cr_2TeI_2 monolayer, and the D_i for the Cr_2TeBr_2 and Cr_2TeCl_2 monolayers is taken the negative value.