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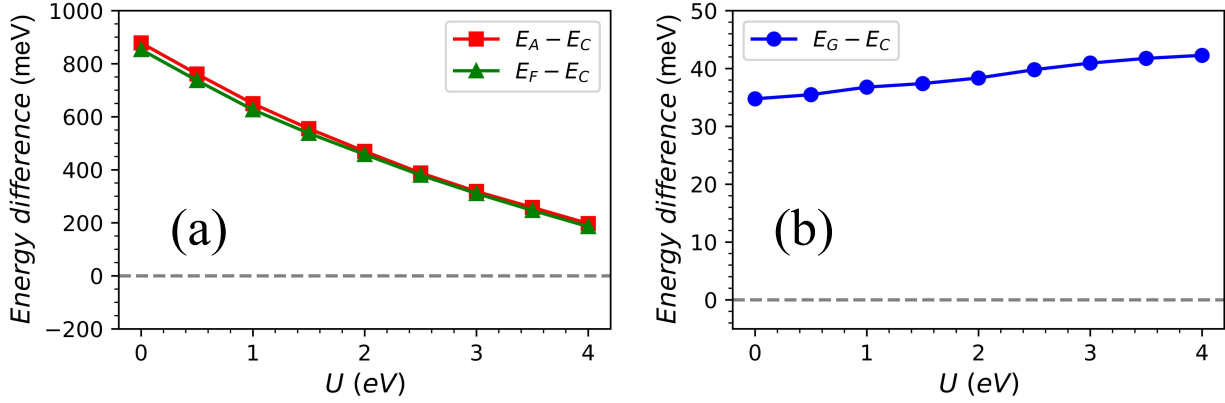


FIG. S1. (Color online) For  $\text{RbCr}_2\text{Se}_2\text{O}$  by considering vdW interaction, the energies (per magnetic primitive cell) of A-, F- and G-type configurations as functions of  $U$ , with C-type set to zero.

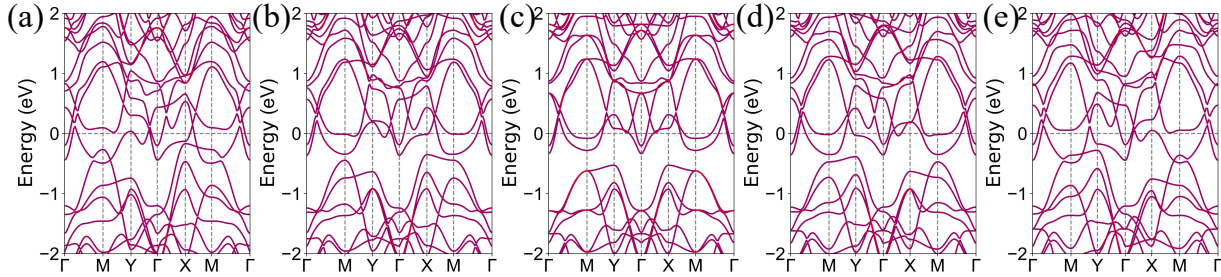


FIG. S2. (Color online) For  $\text{RbCr}_2\text{Se}_2\text{O}$ , the global energy band structure with G-type AFM configuration at  $a/a_0=0.96$  (a), 0.98 (b), 1.00 (c), 1.02 (d) and 1.04 (e). The purple denotes the spin-degenerate bands.

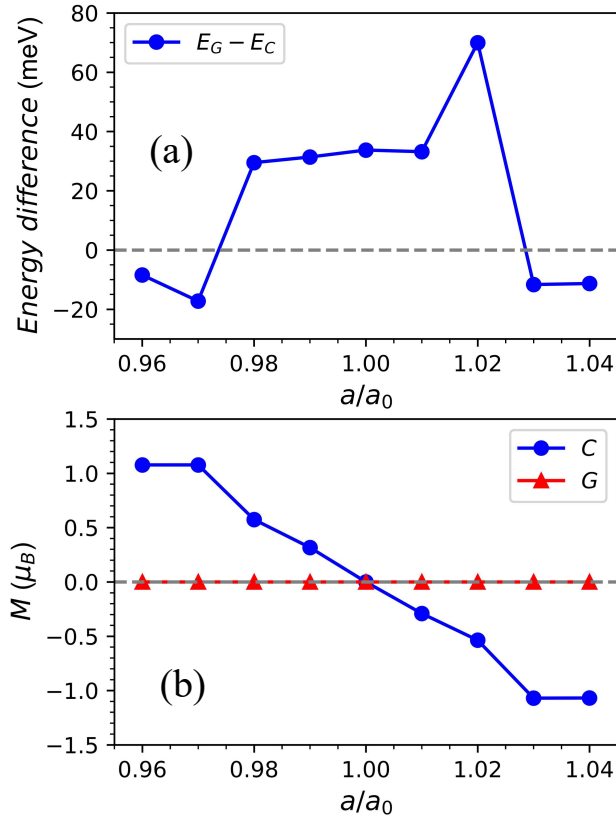


FIG. S3. (Color online) For  $\text{RbCr}_2\text{Se}_2\text{O}$  by GGA+ $U$  ( $U=3.00$  eV), (a): the energy (per magnetic primitive cell) of G-type configuration as function of  $a/a_0$  with C-type set to zero. (b): the total magnetic moment as a function of  $a/a_0$  with C-type and G-type AFM configurations.

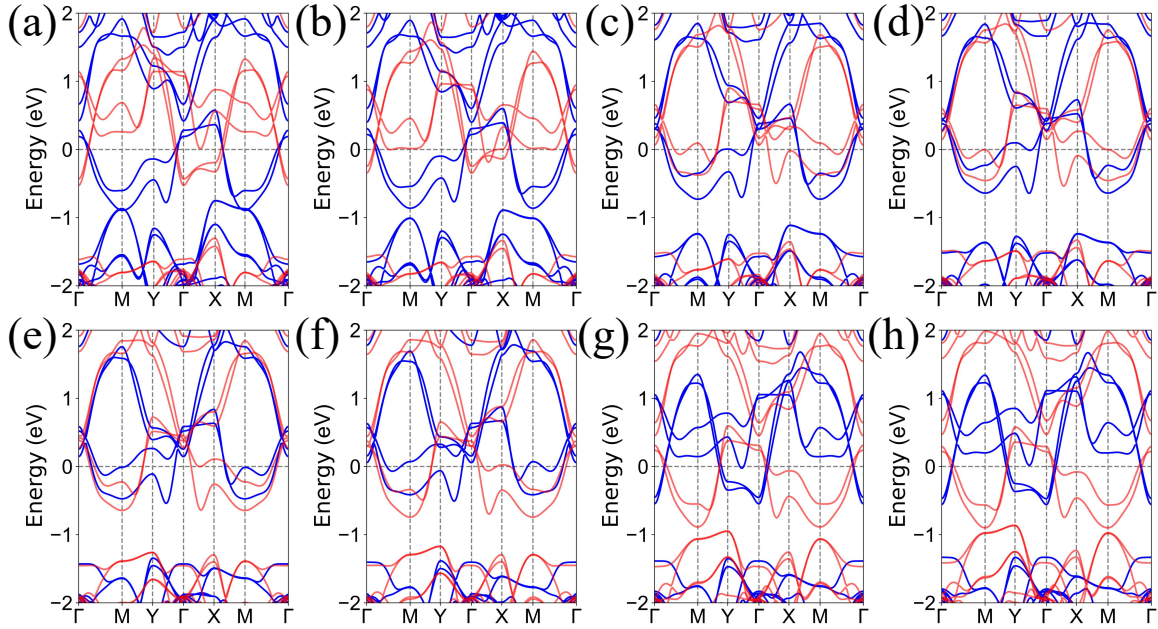


FIG. S4. (Color online) For  $\text{RbCr}_2\text{Se}_2\text{O}$  by GGA+ $U$  ( $U=3.00$  eV), the global energy band structure with C-type AFM configuration at  $a/a_0=0.96$  (a), 0.97 (b), 0.98 (c), 0.99 (d), 1.01 (e), 1.02 (f), 1.03 (g) and 1.04 (h). The blue, red, and purple curves denote the spin-up, spin-down, and spin-degenerate bands, respectively.

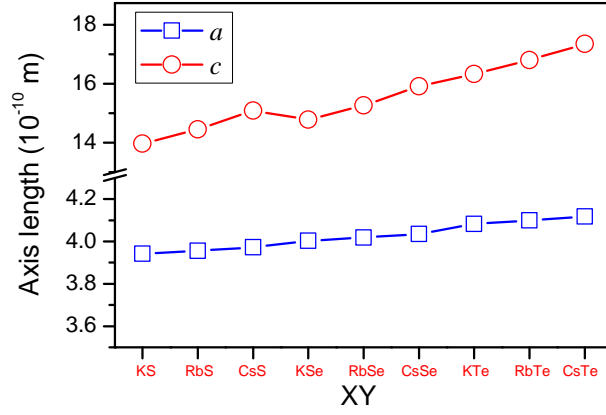


FIG. S5. (Color online) For  $XCr_2Y_2O$  ( $X=K, Rb, Cs$ ;  $Y=S, Se, Te$ ), the dependence of the lattice parameters  $a$  and  $c$  on  $X$  and  $Y$ .

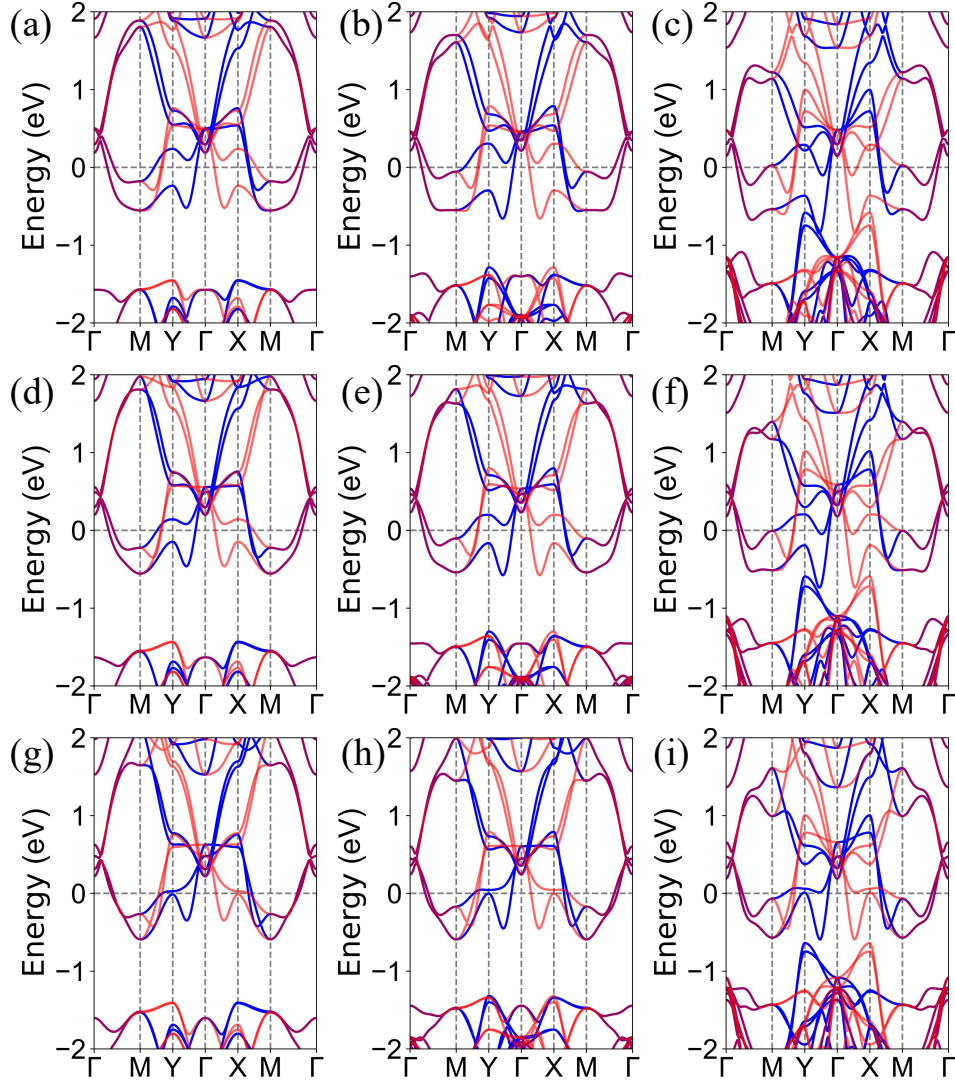


FIG. S6. (Color online) For  $KCr_2S_2O$  (a),  $RbCr_2S_2O$  (b),  $CsCr_2S_2O$  (c),  $KCr_2Se_2O$  (d),  $RbCr_2Se_2O$  (e),  $CsCr_2Se_2O$  (f),  $KCr_2Te_2O$  (g),  $RbCr_2Te_2O$  (h) and  $CsCr_2Te_2O$  (i), the global energy band structure with C-type by using GGA+ $U$  ( $U=3.00$  eV), and the blue, red, and purple curves denote the spin-up, spin-down, and spin-degenerate bands, respectively.