Supplementary Information (SI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2024

#### Supporting Information for

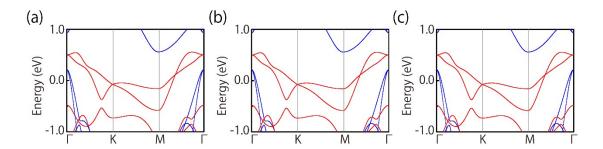
## Multiple Weyl Fermions and Topological Phase Transition in Twodimensional Ferromagnetic CrS<sub>2</sub>

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#### I. Band structures of monolayer CrS2 under different van der Waals corrections



**Figure S1.** (a)-(c) are band structures of monolayer CrS<sub>2</sub> under DFT-D2, DFT-D3 and vdW-DF for van der Waals corrections, respectively. The red and blue lines correspond to the spin-up and spin-down band structures, respectively.

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# ${\color{red} { ext{II. Comparison of the energy among different magnetic states under different $U$} {\color{red} { ext{values}}}$

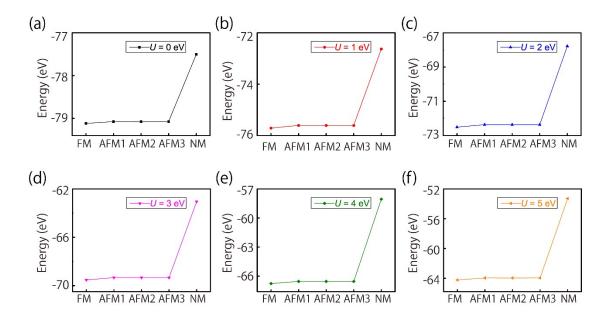
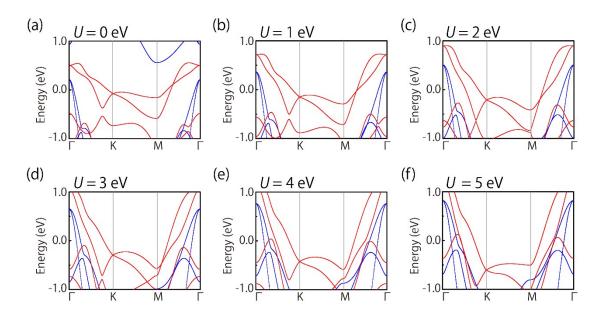


Figure S2. (a)-(f) Comparison of the energy among different magnetic states with U values ranging from 0 to 5 eV.

### **III. Band structures of monolayer CrS<sub>2</sub> under different** *U* **values**



**Figure S3.** The band structures of monolayer  $CrS_2$  when the U values are chosen as (a) 0, (b) 1, (c) 2, (d) 3, (e) 4, and (f) 5 eV. The red and blue lines correspond to the spin-up and spin-down band structures, respectively.