Supporting Information

Insight into the Quantum Anomalous Hall States in Two-Dimensional Kagome Cr_3Se_4 and Fe_3S_4 Monolayers

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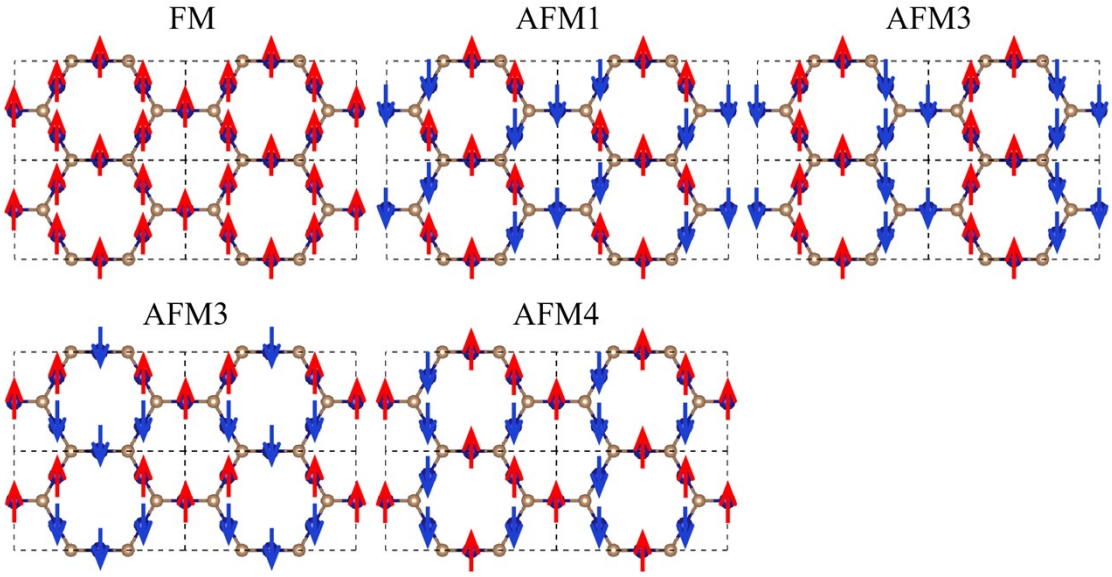

Figure S1. The considered magnetic configurations: ferromagnetic (FM) state and four antiferromagnetic (AFM1, AFM2, AFM3 and AFM4) states for Cr_3Se_4 and Fe_3S_4 monolayers.

Table S1. The relative energy (meV) of Cr_3Se_4 and Fe_3S_4 monolayers with different magnetic states in each formula.

	FM	AFM1	AFM2	AFM3	AFM4
Cr_3Se_4	0	46.1	27.1	44.7	37.4
Fe_3S_4	0	35.1	29.4	34.1	20.9

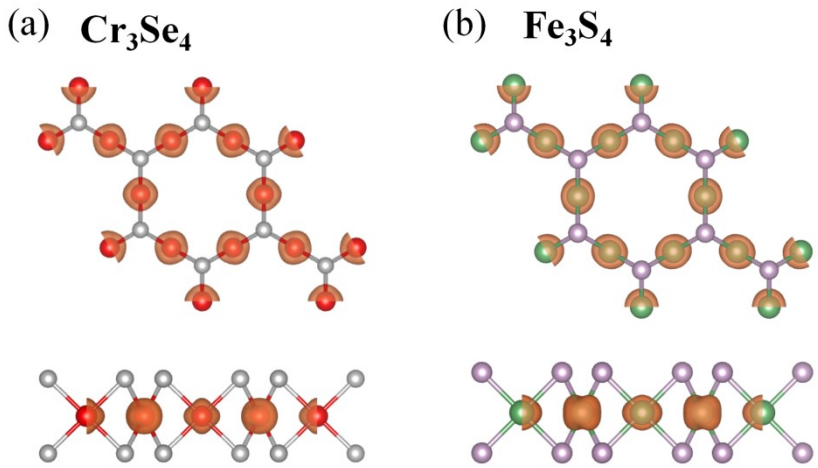

Figure S2. Spin densities of FM Cr_3Se_4 (a) and Fe_3S_4 (b) monolayers.

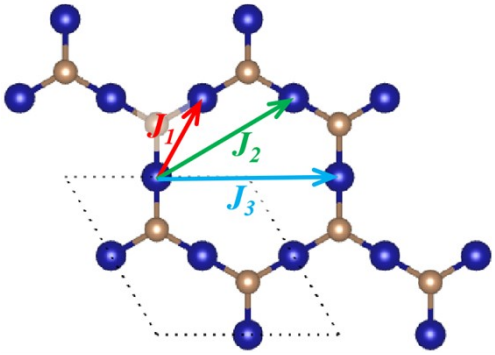

Figure S3. J_1, J_2 and J_3 are the nearest, second-nearest and third-nearest exchange parameters, respectively.

Part I:

The Hamiltonian can be written as below based on 2D Heisenberg Hamiltonian model:

$$H = -\sum_{i,j} J_1 M_i M_j - \sum_{p,q} J_2 M_p M_q - \sum_{m,n} J_3 M_m M_n \qquad (1),$$

where M_i is the magnetic moment of the atom in site i, J_1, J_2 and J_3 denote as the nearest, second-nearest, and third-nearest exchange coupling parameters (as shown in Fig. S3), respectively. The values of J_1, J_2 and J_3 can be estimated from the energy differences between FM and AFM states:

$$E_{FM} = E_0 - (12J_1 + 12J_2 + 18J_3)M^2 \qquad (2),$$

$$E_{AFM1} = E_0 - (-4J_1 - 4J_2 + 10J_3)M^2 \qquad (3),$$

$$E_{AFM2} = E_0 - (-4J_1 + 4J_2 - 6J_3)M^2 \qquad (4),$$

$$E_{AFM3} = E_0 - (-4J_1 - 4J_2 + 6J_3)M^2 \qquad (5),$$

$$E_{AFM4} = E_0 - (4J_1 - 4J_2 - 6J_3)M^2 \qquad (6).$$

The $J_1/J_2/J_3$ values for Cr_3Se_4 monolayer and Fe_3S_4 monolayer are 7.90meV/5.88meV/-8.22meV and 15.6meV/1.33meV/-1.31meV, respectively.

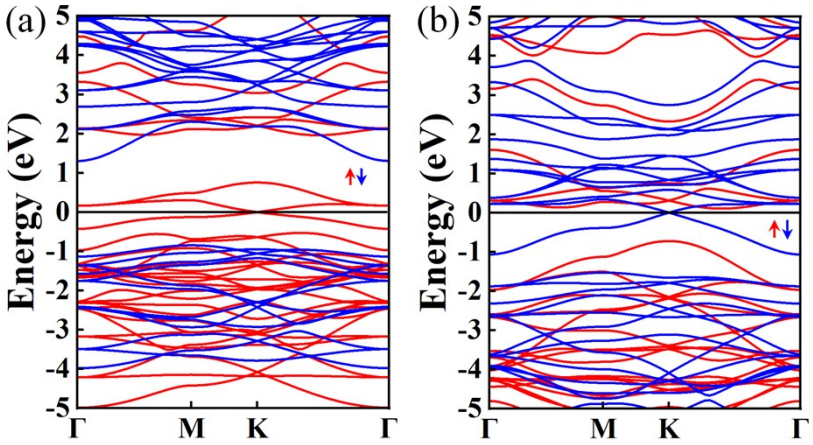

Figure S4. The band structures with large energy window [-5eV, 5eV] of Cr_3Se_4 (a) and Fe_3S_4 (b) monolayers.

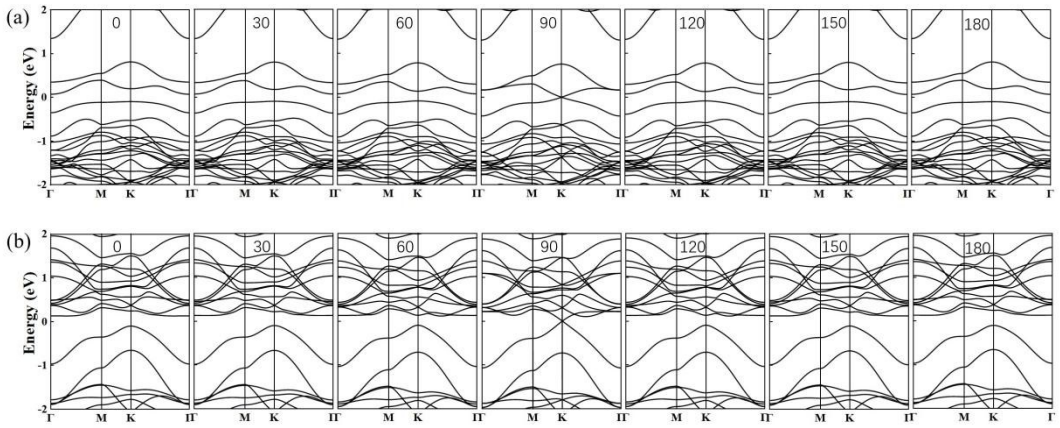

Figure S5. Band structures of Cr_3Se_4 monolayer (a) and Fe_3S_4 monolayer (b) when the *zoy* plane magnetization rotates in the z-direction.

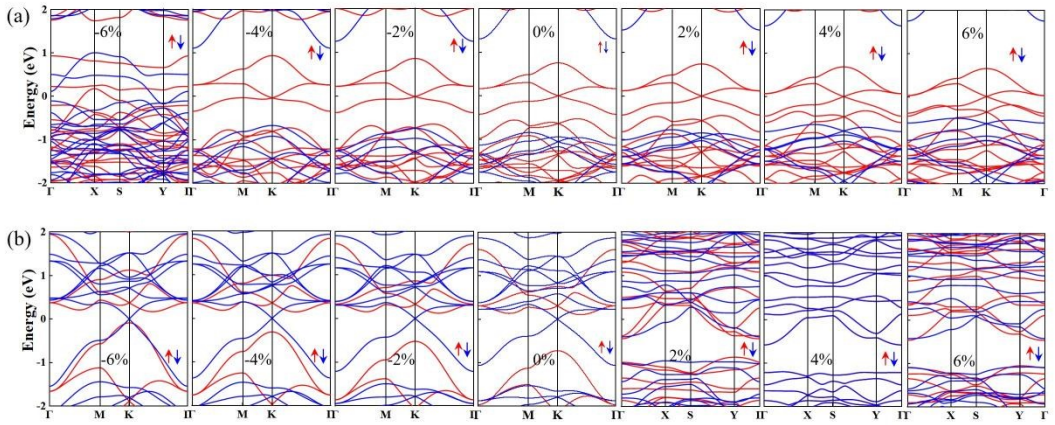

Figure S6. Band structures of Cr_3Se_4 monolayer (a) and Fe_3S_4 monolayer (b) within biaxial tensile/compressive strains of ± 6%.

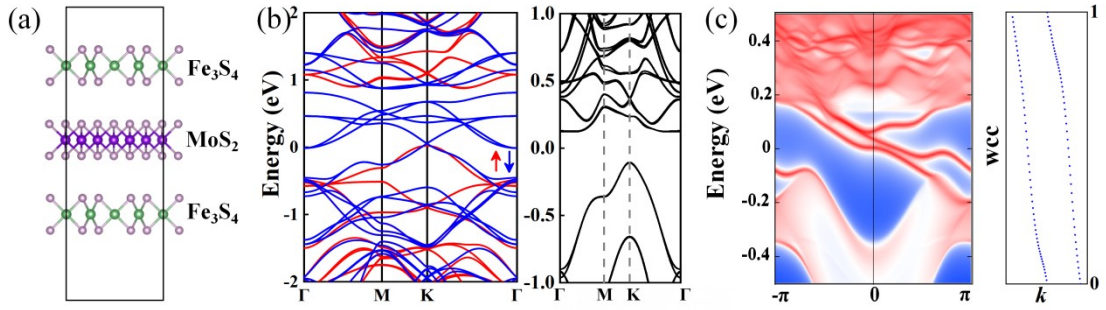

Figure S7. (a) Side view of the $Fe_3S_4/MoS_2/Fe_3S_4$ heterostructures. (b) Spin polarized band structure without SOC and with SOC when magnetization is along *z* direction. (c) Edge states, and wannier charge center (WCC) of $Fe_3S_4/MoS_2/Fe_3S_4$ heterostructure.

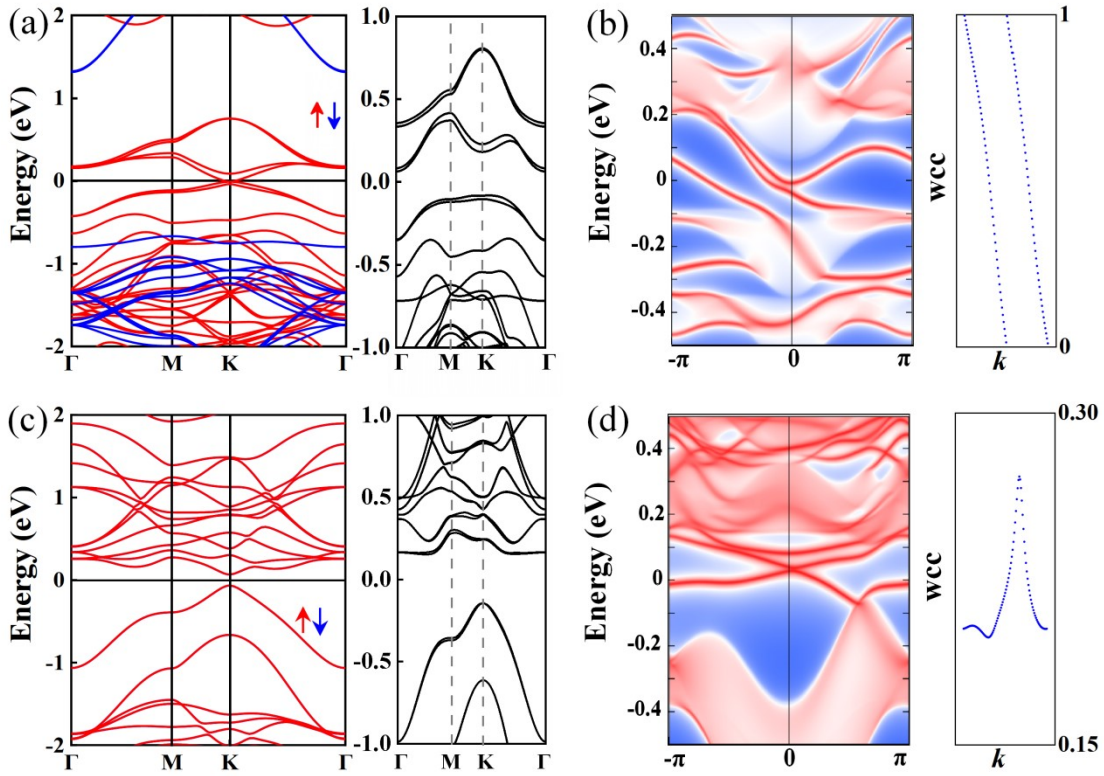

Figure S8. Spin polarized band structures, edge states and wannier charge center (WCC) of bilayer Cr_3Se_4 in the FM (a, b) and bilayer Fe_3S_4 in AFM state (c, d).