Supporting Information for

Fully spin-polarized Weyl fermions and in/out-plane quantum anomalous Hall effects in a two-dimensional d^0 ferromagnet

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I. Spin-down band structures of 1T-YN_2 under different *U* values

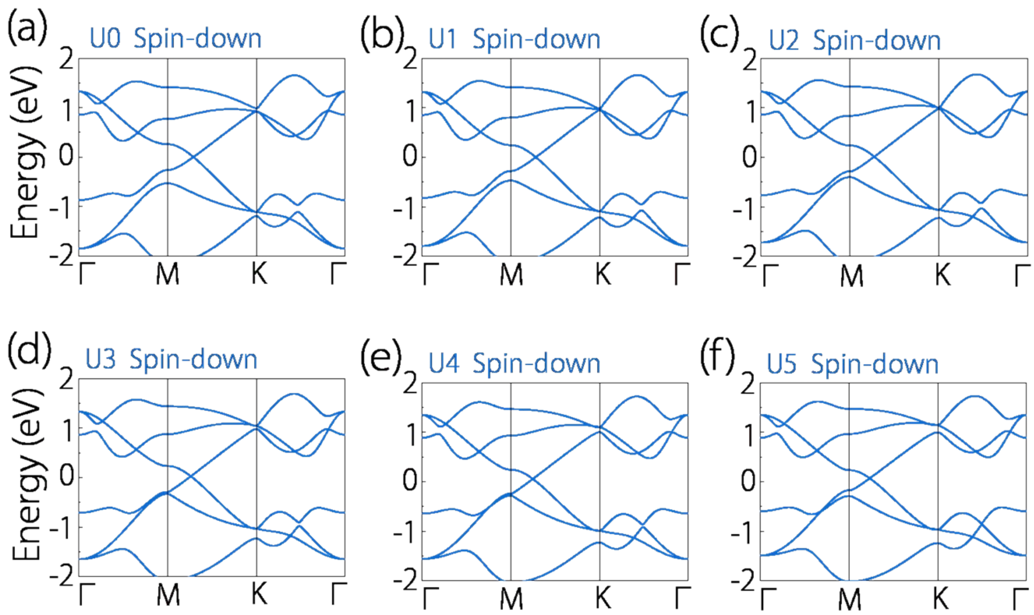

Figure S1. The spin-down band structures of 1T-YN_2 when the *U* values are chosen as (a) 0, (b) 1, (c) 2, (d) 3, (e) 4, and (f) 5 eV. The spin-down band structures not change in a large range of *U* values (0−5 eV).

II. Spin-up band structures of 1T-YN_2 under different *U* values

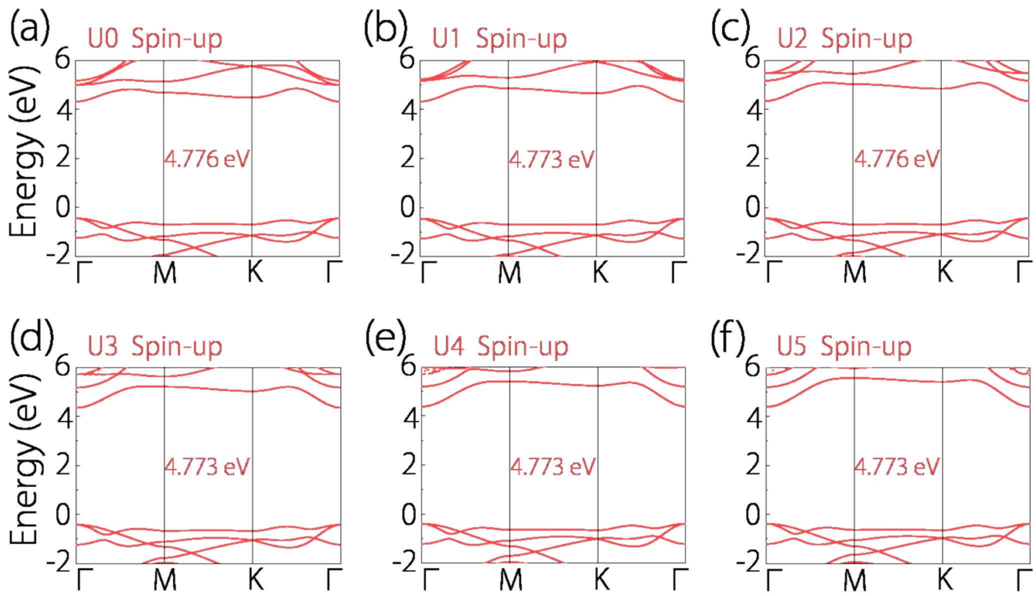

Figure S2. The spin-up band structures of 1T-YN_2 when the *U* values are chosen as (a) 0, (b) 1, (c) 2, (d) 3, (e) 4, and (f) 5 eV. The spin-up band structures and gap values not change in a large range of *U* values (0−5 eV).

II. The lattice structure, band structure with/without SOC and edge states of the YN_2/GaSe heterostructures

The lattice constant of the GaSe monolayer (3.82 Å) is close to that of 1T-YN_2 (3.76 Å), therefore it is expected to be a suitable substrate. The lattice structure of YN_2/GeSe heterostructure is shown in Figure S3(a) and (b). It exhibits a hexagonal structure and has the space group *P3m1.* The interlayer distance (*h*) between the two monolayers is 2.943 Å. The lattice constant for YN_2/GeSe heterostructure is optimized as a = b = 3.776 Å, and the Y-N, N-N, Ga-Se, Ga-Ga bond length are 2.377Å, 2.863 Å, 2.485Å, 2.452 Å, respectively. We calculate the band structure and edge state of YN_2/GeSe heterostructure, and the results show that YN_2/GeSe heterostructure can retain nontrivial topological properties with in-plane QAHE (see Figure S3). The Chern number takes values alternating between +1, 0 and -1 for the in-plane QAHE phases, as shown in Figure S3(f). Here, we show the corresponding topological edge states for φ=0° and φ=180° in Figure S3(h) and (i), respectively. In the energy window of SOC gap, we can observe one edge state connecting the valence and conduction band for each edge, characterizing the nontrivial band topology for the QAHE phase. In addition, we can observe that the edge state for φ=0° and φ=180° shows opposite orientations. These results indicate that the in-plane QAHE is robust against the interaction between 1T-YN_2 and substrate.

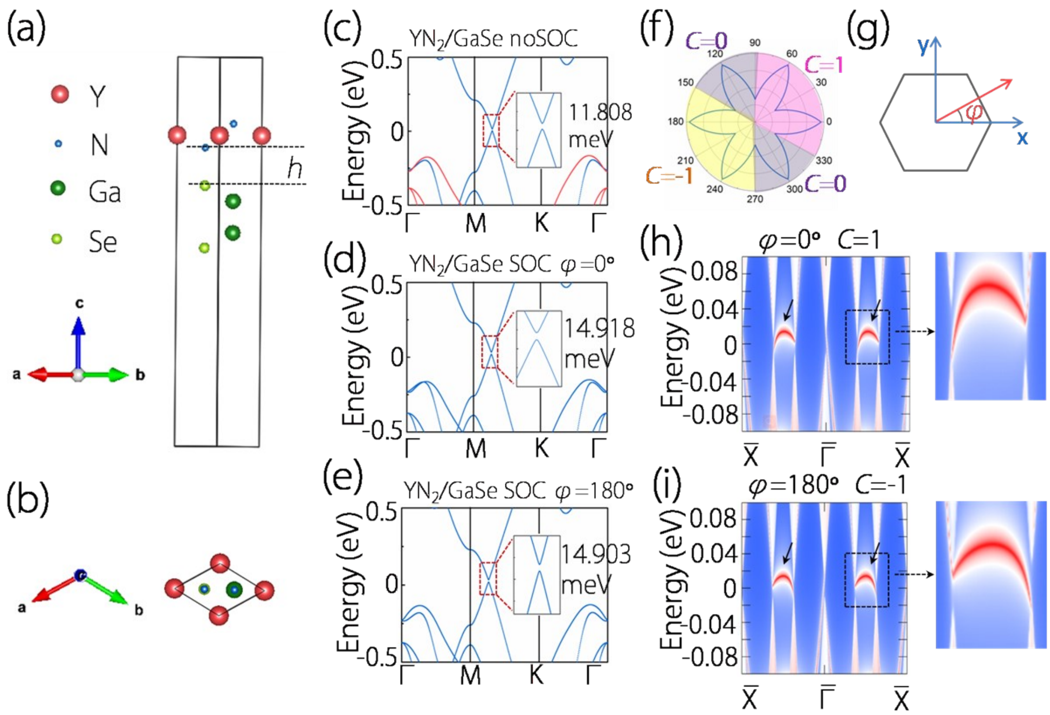

Figure S3. (a) Side view of the YN_2/GaSe heterostructure along (1-10) direction. *h* indicates the interlayer distance. (b) Vertical view along (001) direction of the heterostructure. (c) The band structures of YN_2/GaSe heterostructure without SOC. The spin up band structure is plotted with red dots and the spin down band structure is given by blue dots. The insets demonstrate the band gap. (d) and (e) are the band structures of YN_2/GaSe heterostructure under SOC with in-plane magnetization along $\varphi = 0°$ and $\varphi = 180°$ in (g), respectively. (f) The flowerlike curve (the blue line) shows the band gap as a function of the azimuthal angle φ for the magnetization direction. The polar radius represents the gap value. The pink, purple and yellow indicates the regions with Chern number $C = +1$, 0 and -1. (h) and (i) are the one-dimensional topological edge states (pointed by arrows), showing the QAHE state with in-plane magnetization along $\varphi = 0°$ and $\varphi = 180°$. (h) and (i) manifest opposite edge states.