Supplemental Materials for "Quantum anomalous Hall effect in germanene by proximity coupling to a semiconducting ferromagnetic substrate NiI_2"

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ELECTRONIC CORRELATION (*U*) AND BAND STRUCTURES

In the range of *U* from 3 to 5 eV, the lattice constants yield good comparison with the experimental value of bulk NiI_2, 3.90 Å. When *U* increases, due to the stronger repulsion of localized electronic states, the μ_{Ni} and E_{gap} both increase. Notably, the I atoms are spin polarized due to the magnetic proximity of Ni atoms. These basic properties of ML-NiI_2 in previous works are also provided in Table SI. Notably, a, μ_{Ni}, μ_I, and E_{gap} in our work when *U* = 4 eV is very similar to the results in Ref.[1].

TABLE SI. The optimized lattice constants a, magnetic moments of Ni μ_{Ni} and I μ_I, band-gap energy E_{gap}.

U (eV)	a (Å)	μ_{Ni} (μ_B)	μ_I (μ_B)	E_{gap} (meV)
3	3.98	1.35	0.21	40.88
4	3.98	1.42	0.19	19.01
5	3.99	1.49	0.17	16.4

INTERLAYER CHARGE TRANSFER IN Ge/NiI_2 FM HTS

In order to confirm the interlayer charge transfer of Ge/NiI_2 HTS, we further calculate the work functions, differential charge density, and perform the Bader charge analysis. As shown in Figs. S1(a)-(c), the work functions of germanene, ML-NiI_2, and Ge/NiI_2 FM HTS are 4.52, 5.65, and 4.67 eV, respectively. The smaller work function of germanene compared with ML-NiI_2 indicates that the electrons can flow from germanene to ML-NiI_2 when germanene comes into contact with ML-NiI_2, see Fig. S1(d). As a result, the ML-NiI_2 gathers negative charges, while germanene accumulates positive charges, which is consistent with the above analysis about the hole doping in germanene and electron doping in ML-NiI_2. Moreover, the electrons in the germanene can spontaneously flow into the adjacent ML-NiI_2 to achieve a balanced work function, thus leading to a vertical built-in electric field between two layers. Note that the previous study indicated that the vertical electric field combining with a magnetic field can significantly increase the valley-splitting in germanene[2]. Therefore, our proposed 2D FM vdW HTS subject to magnetic fields are expected to further enhance the valley-splitting due to cooperative effects of their intrinsic FM and electric fields. In Fig. S1(c), we also draw the 3D differential charge density of HTS in order to directly observe the charge transfer at the interface of HTS. The yellow and cyan areas represent electron accumulation and depletion, respectively, which can induce the built-in electric field at the interface, pointing from germanene to ML-NiI_2. Also, the Bader charge analysis, a quantitative analysis, is performed in the Ge/NiI_2 HTS, which shows that 0.026 electrons transfer from the germanene to the ML-NiI_2. We expect that the interlayer charge transfer in Ge/NiI_2 can be confirmed through the above method. Thus, the interlayer charge transfer in Ge/NiI_2 FM HTS is confirmed by different methods, suggesting the correctness of our results.

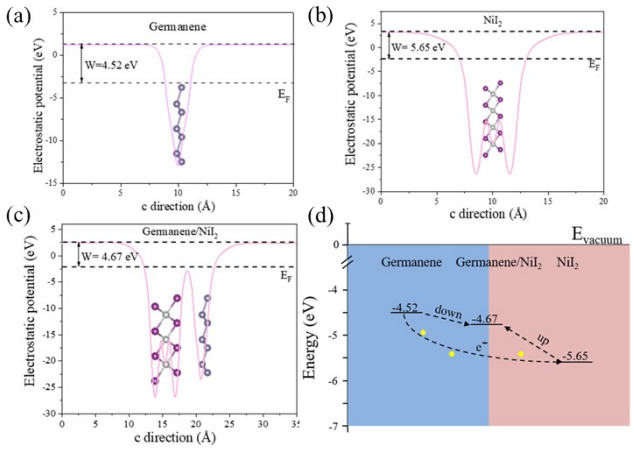

FIG. S1. The electrostatic potential of (a) germanene, (b) ML-NiI_2 and (c) Ge/NiI_2 FM HTS. (d) The transfer direction of electrons and the movement of the E_F in the process of forming HTS. The yellow and cyan areas represent electron accumulation and depletion, respectively, and the black arrows represent the direction of built-in electric field.

MAGNETIC ANISOTROPY TUNED BY INTERLAYER SPACING

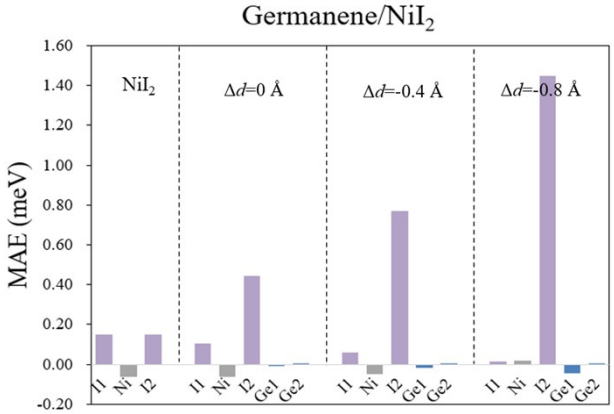

FIG. S2. The layer-resolved MAE of ML-NiI_2 and Ge/NiI_2 with Δd = 0, −0.4, and −0.8 Å, respectively.

TABLE SII. The matrix differences between magnetization along z [001] and x [100] in *Eqs.* (1) and (2). u^-, o^+, and o^- represent unoccupied spin-down states, occupied spin-up and spin-down states, respectively.

		o^+			o^-	
u^-	p_y	p_z	p_x	p_y	p_z	p_x
p_y	0	1	-1	0	-1	1
p_z	1	0	0	-1	0	0
p_x	-1	0	0	1	0	0

References:

1 M. Lu, Q. Yao, C. Xiao, C. Huang and E. Kan, Mechanical, Electronic, and Magnetic Properties of NiX 2 (X = Cl, Br, I) Layers, *ACS Omega*, 2019, **4**, 5714–5721.

2 Z. Jiao, Q. Yao, A. N. Rudenko, L. Zhang and H. J. W. Zandvliet, Germanium/MoS2: Competition between the growth of germanene and intercalation, *Phys. Rev. B*, 2020, **102**, 205419.