

Supplemental Material for

Two-dimensional antiferromagnetic topological insulator in KCuSe/NaMnBi van der Waals heterobilayers

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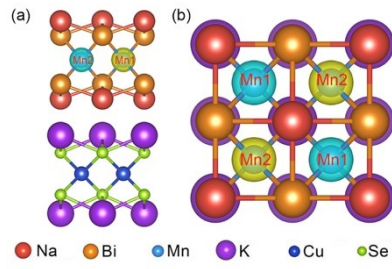


Fig. S1 Calculated isosurfaces of spin density functions in real space for KCuSe/NaMnBi van der Waals heterobilayers showing (a) side and (b) top views in square lattice.

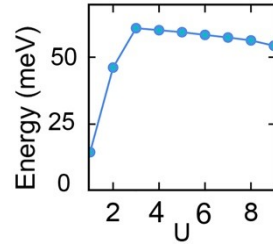


Fig. S2 Variation of the energy gaps for KCuSe/NaMnBi heterobilayer in AFM state with SOC. For the whole U interval from 1 to 9, the material remains topologically nontrivial.

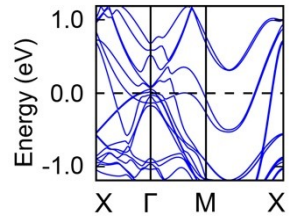


Fig. S3 Band structure of KCuSe/NaMnBi heterobilayer in ferromagnetic state with SOC. The Fermi level is indicated with a dashed horizontal line.

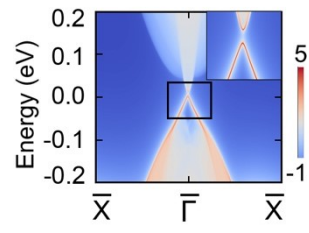


Fig. S4 Edge state of AFM KCuSe/NaMnBi heterobilayer with a termination of FM order. A small gap is clearly seen.

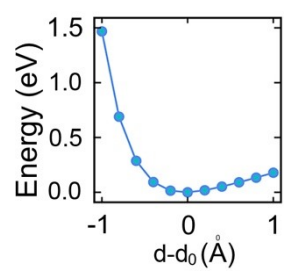


Fig. S5 The relative energies versus the variation ($d - d_0$) in the separation between KCuSe and NaMnBi QLs. The total energy of the ground state with $d_0 = 2.56 \text{ \AA}$ was set as 0 eV.