Supplemental Material

Possible realization of high-temperature and multichannel quantum anomalous Hall effect in graphene/$CrBr_3$ heterostructures under pressure

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Supporting Note I: three typical configurations of Gr/$CrBr_3$ heterobilayers

Here, we mainly considered three typical configurations of Gr/$CrBr_3$ heterobilayers, as displayed in Fig. S1. Fig. S1(d) gives the corresponding total energies of configurations (a)-(c) (denoted as (I)-(III), respectively). Due to configuration (I) harboring the lowest energies, this configuration is adopted for calculations in the main text. Our calculations show that the average inter-layer distances are ~3.5 Å for all of the three heterobilayers, indicating the interfacial coupling between graphene and $CrBr_3$ monolayer indeed belongs to vdW interaction.

Supporting Note II: band structures and topological properties of the other two configurations

The band structures of configurations (II) and (III) under the pressure of ~6.5 GPa (the layer distance is ~2.7 Å) are shown in Fig. S6. Obviously, Dirac cones of graphene are also spin-polarized (see Fig. S6 (a) and (e)). When SOC is considered, a

band gap opens at either the K and K' points, as illustrated in Fig. S6(b) and (f). Fig. S6(c,d) and (g,h) zoom in on the band structures of Fig. S6(b) and (f) near the K and K' points, respectively. The global band gaps with 10.6 and 8.7 meV locate near E_F for configurations (I) and (II), respectively. The Berry curvatures calculations (see Fig. S7) demonstrate that the SOC-induced band gaps for configurations (II) and (III) are topological nontrivial. By integrating the Berry curvatures, a nonzero Chern number of C = -2 is obtained for each of configuration (II) and (III), corresponding to the quantized Hall conductance of $\sigma_{xy} = -2e^2/h$. All those suggest that Gr/$CrBr_3$ heterobilayer can be converted into a QAHE system under pressure.

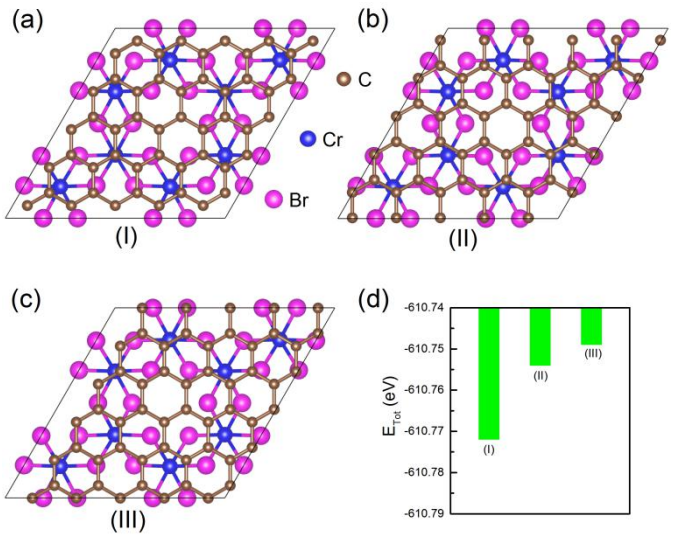

Fig. S1 (a)-(c) Top views of three typical configurations of Gr/$CrBr_3$, denoted as (I)-(III). (d) The corresponding total energies of configurations (I)-(III), respectively. The configuration (I) is adopted for calculations in the main text.

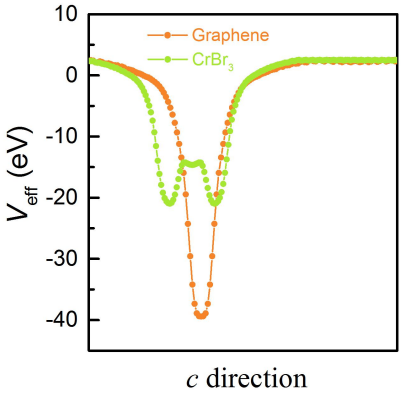

Fig. S2 The electrostatic potential V_{eff} of monolayer $CrBr_3$ (green dotted line) and graphene (yellow dotted line). The vacuum level E_{vac} of $CrBr_3$ and graphene are 2.90 eV and 2.54 eV. The calculated E_F of $CrBr_3$ and graphene are -1.72 eV and -3.94 eV without SOC, respectively.

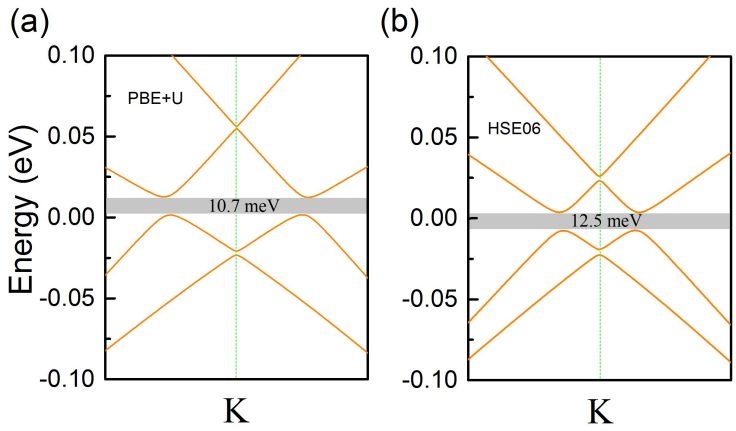

Fig. S3 Calculated band structures of Gr/$CrBr_3$ heterobilayer at a pressure of 6.5 GPa by using PBE+U (a) and HSE06 (b) functionals.

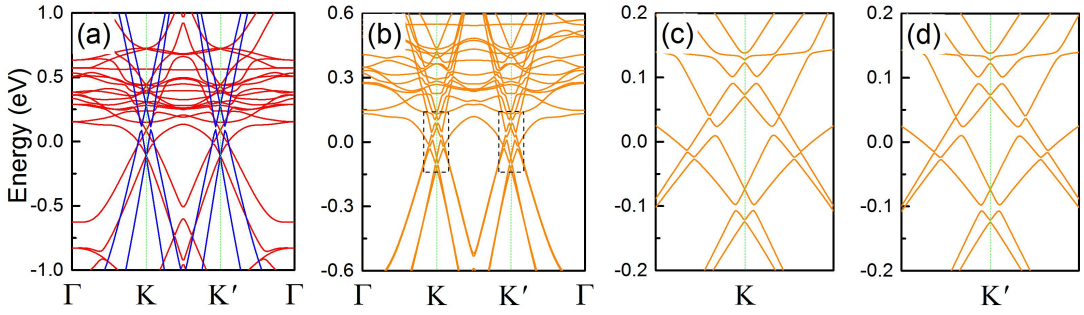

Fig. S4 Band structures of Gr/$CrBr_3$/Gr sandwiched heterostructure without (a) and with (b) SOC at a pressure of 4.8 GPa, with the red and blue lines representing the spin-up and spin-down bands, respectively. (c) and (d) are the zoom-in views of K and K' points near E_F in (b).

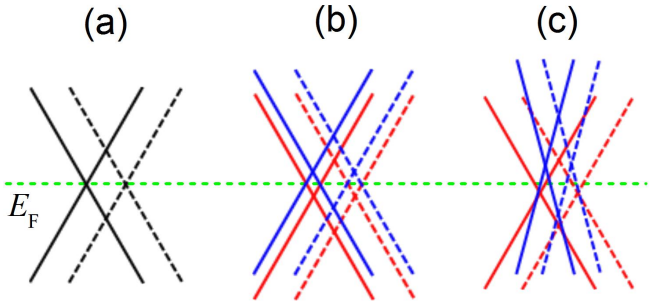

Fig. S5 The schematic band evolution of Gr/$CrBr_3$/Gr system. (a) Two Dirac cones coexit at the K (K') point in the heterostructure. (b) two Dirac cones split into two pairs of spin-up (red colors) and spin-down (blue colors) Dirac cones when magnetism is introduced. (c) pressure-induced the shift of the spin-down Dirac cones, where cross points of spin-up and spin-down bands do not locate on a line. Here, the solid and dashed lines represent the Dirac cones of top and bottom layer of graphene in Gr/$CrBr_3$/Gr system. The green dashed line denotes Fermi level (E_F).

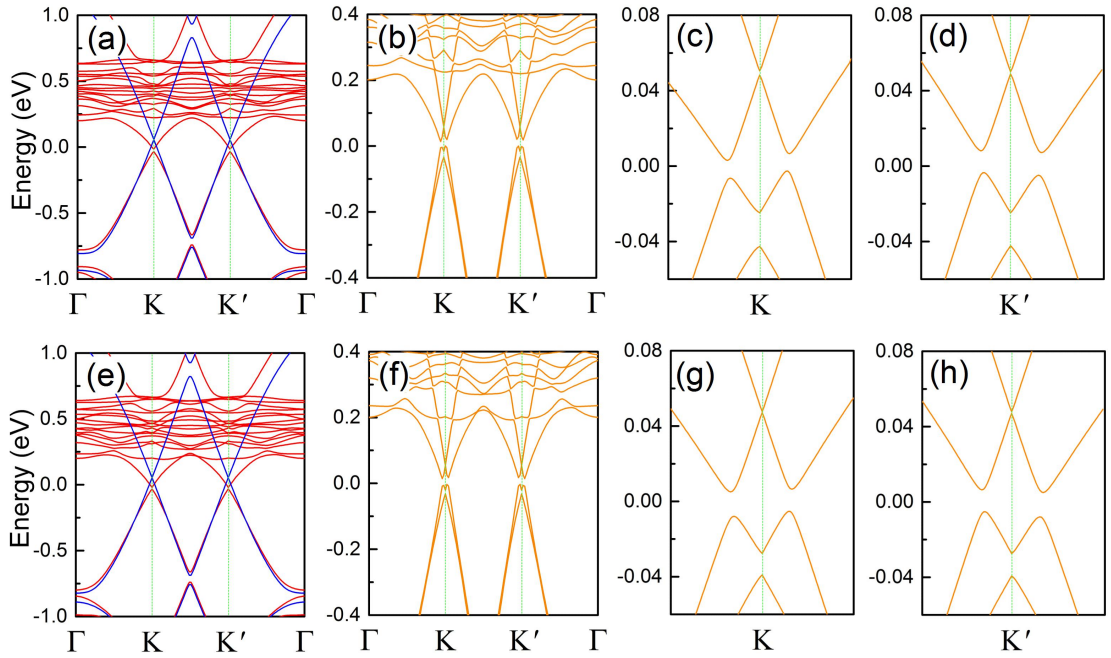

Fig. S6 Band structures of configurations (II) (a)-(d) and (III) (e)-(h) of Gr/$CrBr_3$ heterobilayers (Fig. S1) under pressure, respectively. (a),(b) and (e),(f) denote the band structures without and with SOC. The red and blue lines represent the spin-up and spin-down bands. (c),(d) and (g),(h) are the zoom-in views of K and K' points near E_F in (b) and (f).

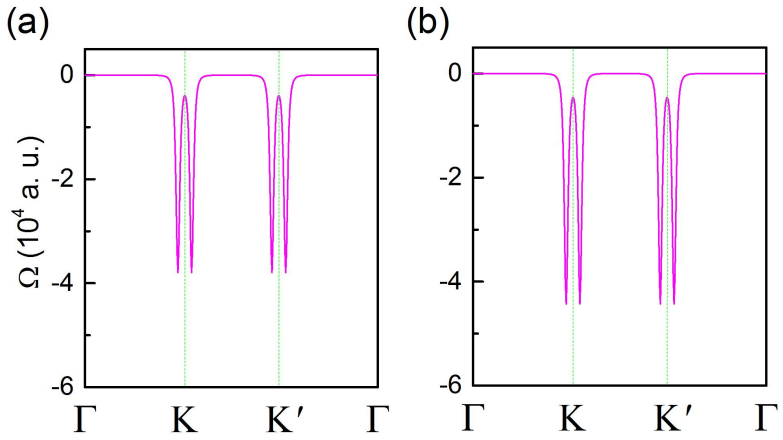

Fig. S7 Corresponding Berry curvatures of configurations (II) (a) and (III) (b) in Fig. S1, respectively.