Electronic Supplementary Material (ESI) for Nanoscale.

Supplemental Material

High-temperature and multichannel quantum anomalous Hall effect in pristine and alkali-metal-doped $CrBr_3$ monolayers

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Supporting note 1. Topological states of electron-doped $CrBr_3$ monolayer

Our calculated results in the main text have demonstrated that the topologically nontrivial band gap of monolayered $CrBr_3$ locates far above the Fermi level, indicating that the topological states can not be directly observed in the experiment. Our further calculations have shown that the Fermi level can be tuned into the band gap via one electron doping per unit cell, the corresponding doping concentration is ~2.8×10^{14} cm^{-2}. Fig. S1 gives the band structure of electron-doped $CrBr_3$ monolayer with considering of spin-orbit coupling (SOC). Obviously, a global band gap of 12.3 meV is achieved in the electron-doped system. The calculated band structure obtained from Wannier interpretation is nearly the same as that obtained from DFT calculations. Similar to the pristine $CrBr_3$, both positive and negative Berry curvatures appear along the high symmetry path. By integrating these nontrivial Berry curvatures over the first BZ, a high Chern number of $C = 2$ is again obtained, demonstrating the topological properties of pristine $CrBr_3$ can be well preserved by means of electron-doping.

Supporting note 2. Hubbard *U* effects on the band gap of the pristine $CrBr_3$ and alkali-metal-doped $CrBr_3$

In order to better describe the Cr 3*d* electrons, the GGA + *U* method was employed. The effective Hubbard *U* effects on the SOC-induced band gap and topological properties of the pristine and alkali-metal-doped $CrBr_3$ are investigated for pristine and alkali-metal-doped $CrBr_3$ monolayer, as shown in Fig. S4. Although *U* affects the quantitative value of the band gap, it does not alter the central physics of this study, suggesting the robustness of the topological states in all systems, especially in the alkali-metal-doped $CrBr_3$ systems.

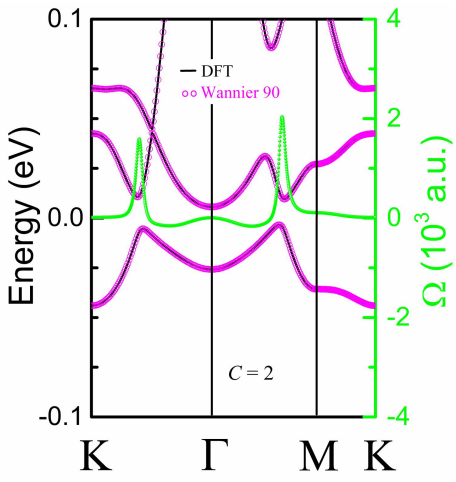

Fig. S1 The band structure of one-electron-doped $CrBr_3$ monolayer with SOC using the DFT calculations (solid black curves) and Wannier interpretation (open magenta circles). The green dots denote the Berry curvature (in atomic units (a.u.)).

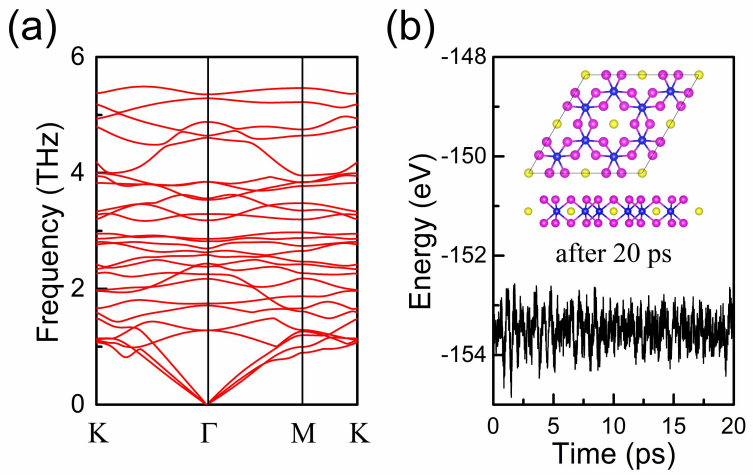

Fig. S2 (a) Calculated phonon spectra of a Na-doped $CrBr_3$ monolayer. (b) AIMD simulations of a Na-doped $CrBr_3$ monolayer at 300 K. The insets in (b) display the final structure after 20 ps.

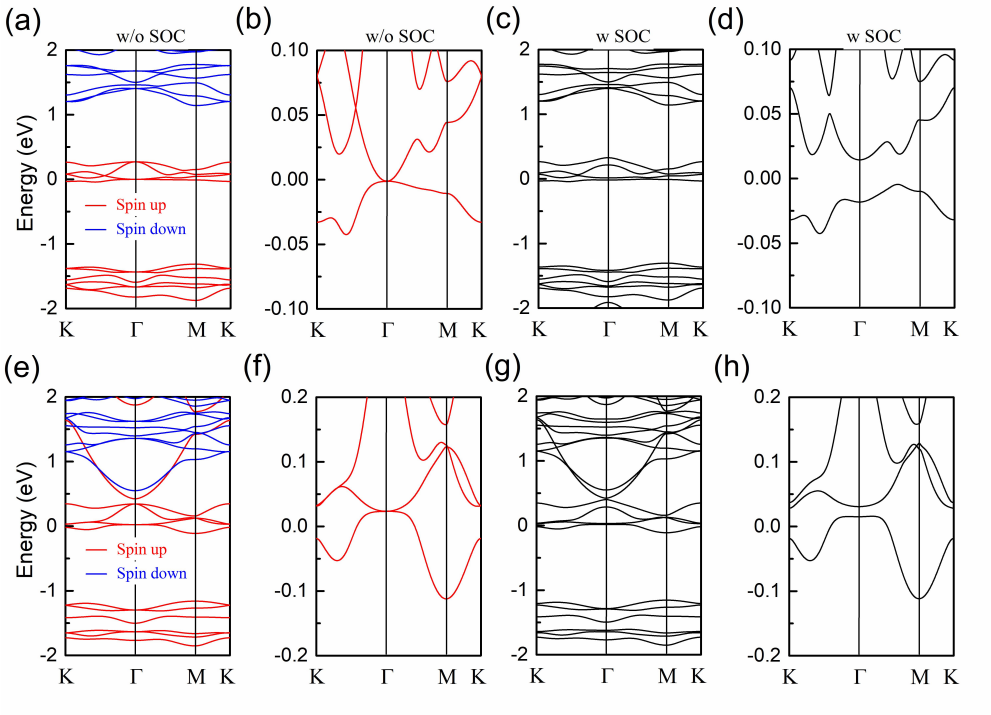

Fig. S3 Band structures of a Li-doped $CrBr_3$ monolayer without (a) and with SOC (c). The red and blue lines in (a) represent spin-up and spin-down bands, respectively. (b) and (d) are the magnified bands near Fermi level in (a) and (c). (e)-(h) The same as (a)-(d) but for a K-doped $CrBr_3$ monolayer.

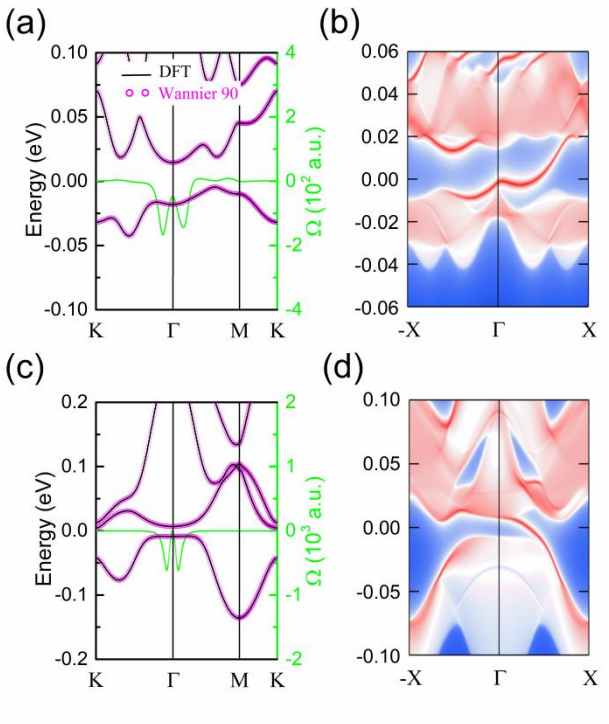

Fig. S4 (a) Calculated band structures of a Li-doped $CrBr_3$ monolayer with SOC using the DFT calculations (solid black curves) and Wannier interpretation (open magenta circles). The green dots denote the Berry curvature (in atomic units (a.u.)). (b) Calculated edge states of a half-infinite monolayer. (c) and (d) The same as (a) and (b) but for a K-doped $CrBr_3$ monolayer.

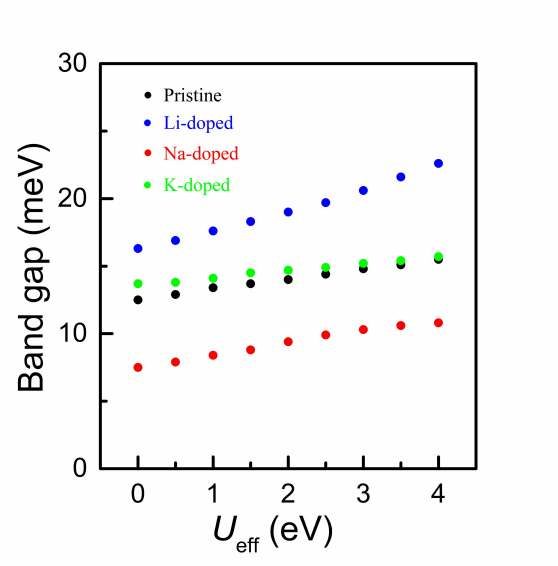

FIG. S5 Hubbard *U* effects on the nontrivial band gaps of pristine and alkali-metal-doped $CrBr_3$ monolayer.

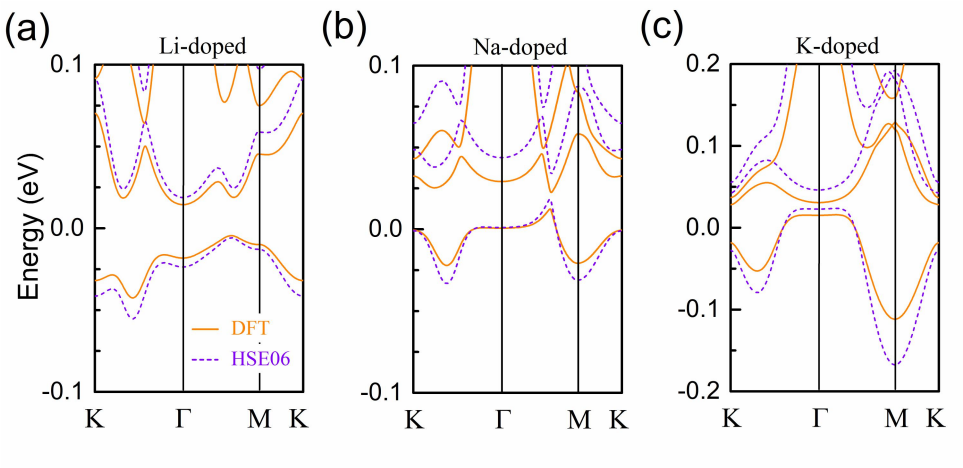

FIG. S6 Calculate band structures of Li (a), Na (b), and K (c)-doped $CrBr_3$ monolayers using DFT+*U* and HSE06 method.