supplementary material:

Combined piezoelectricity, valley splitting and Dzyaloshinskii-Moriya interaction in

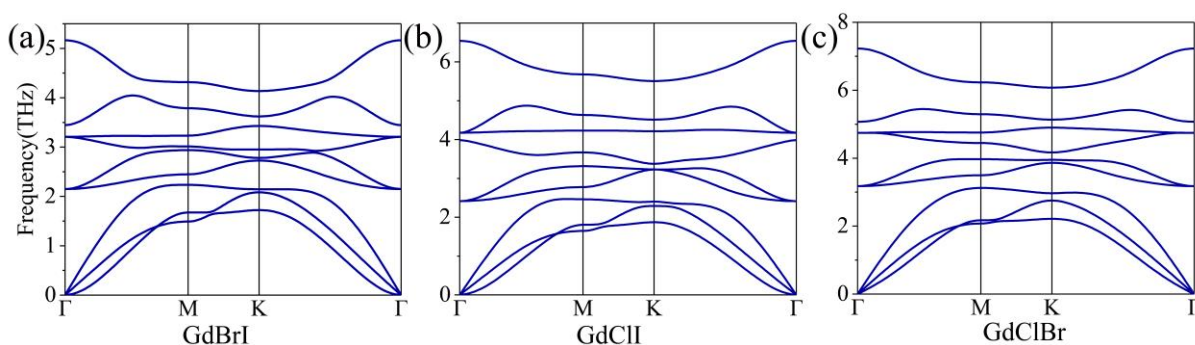**Janus Gd*XY* (*X*, *Y* = Cl, Br, I) magnetic semiconductors**

Fig. S1. The phonon spectrum of monolayer GdBrI (a), GdClI (b), and GdClBr (c).
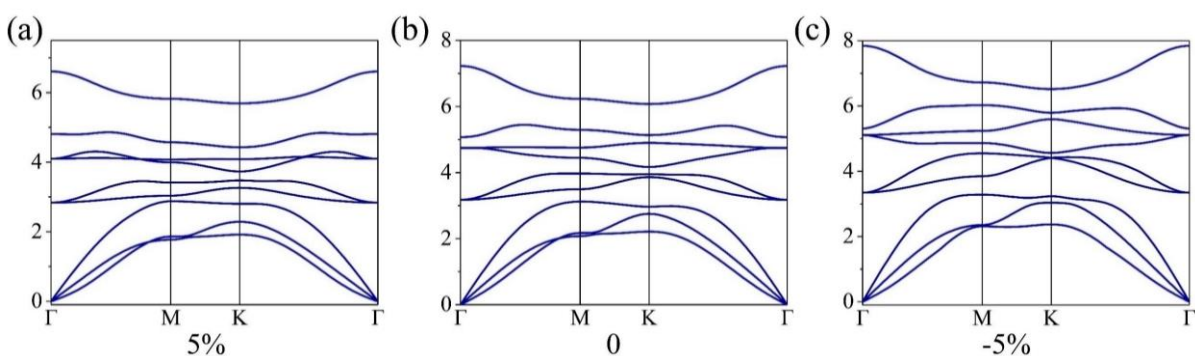

Fig. S2. The phonon spectrum of monolayer GdClBr with biaxial strain of -5% (a), 0(b) and 5% (c).
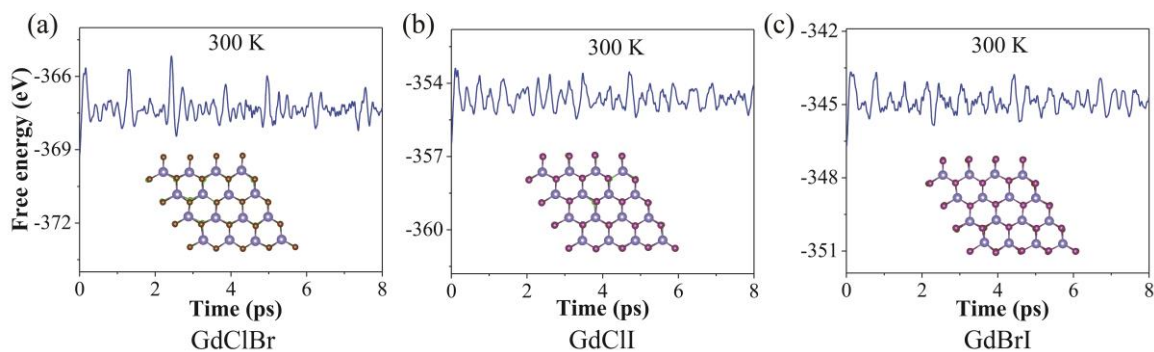

Fig. S3. The variation of total free energy during the 8 ps ab initio molecular dynamics simulation of

monolayer GdClBr (a), GdClI (b), and GdBrI (c). The inset show the final structure after 8 ps at 300
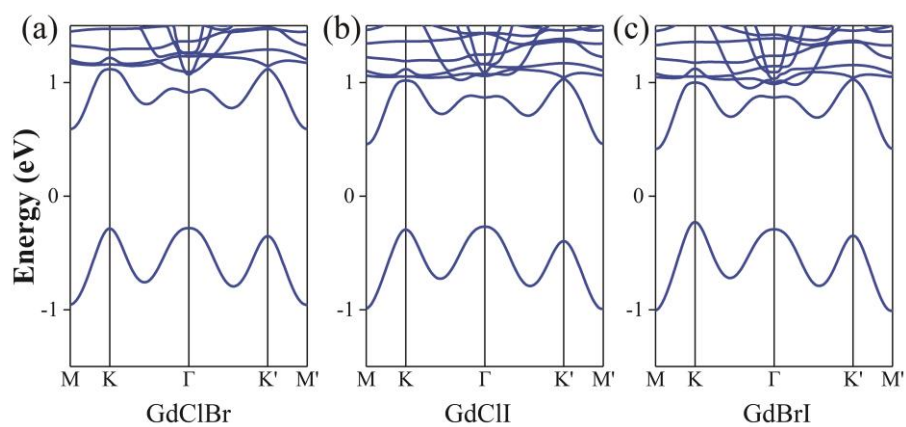
K.

Fig. S4. The band structure with SOC near the Fermi level of monolayer GdClBr (a), GdClI (b), and
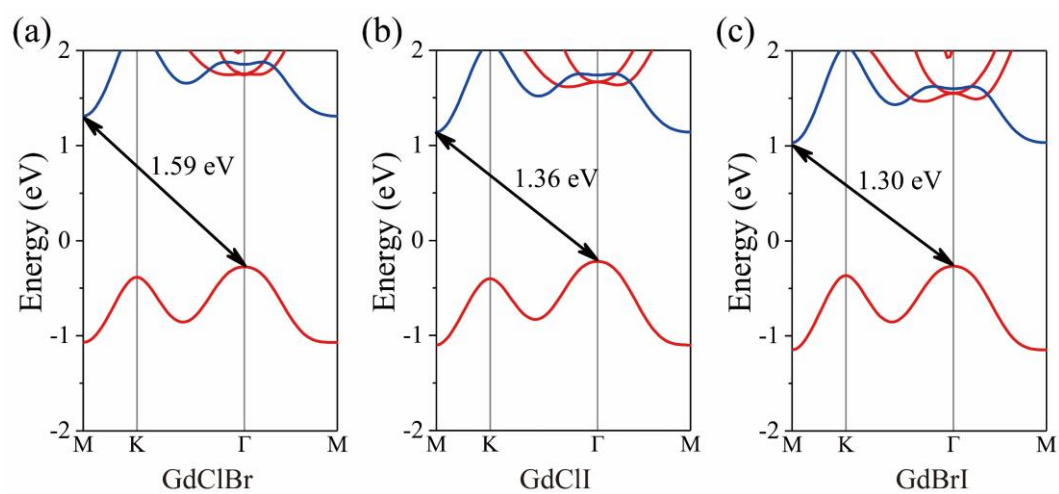
GdBrI (c).

Fig. S5.The band structure calculated by HSE06 with hybrid functional of monolayer GdClBr (a), GdClI
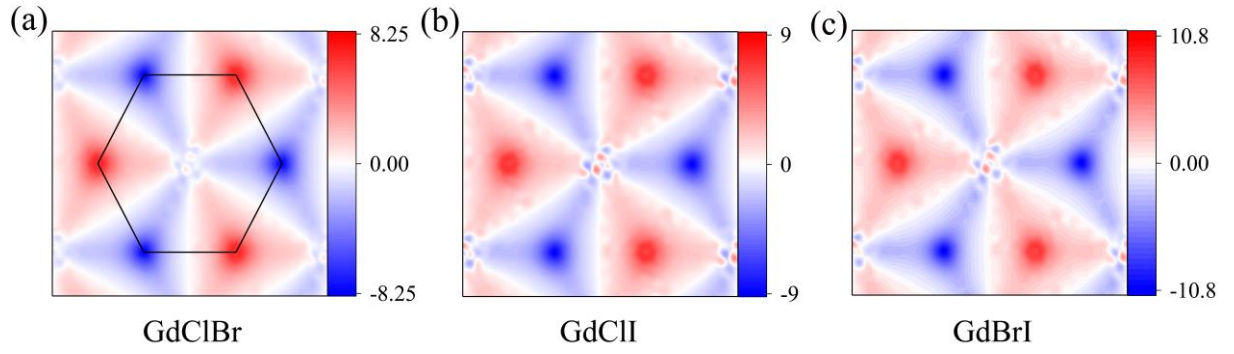
(b), and GdBrI (c).

Fig. S6. The Berry curvatures at the top valence-band of 2D Brillouin zone of monolayer GdClBr (a), GdClI (b), and GdBrI (c).
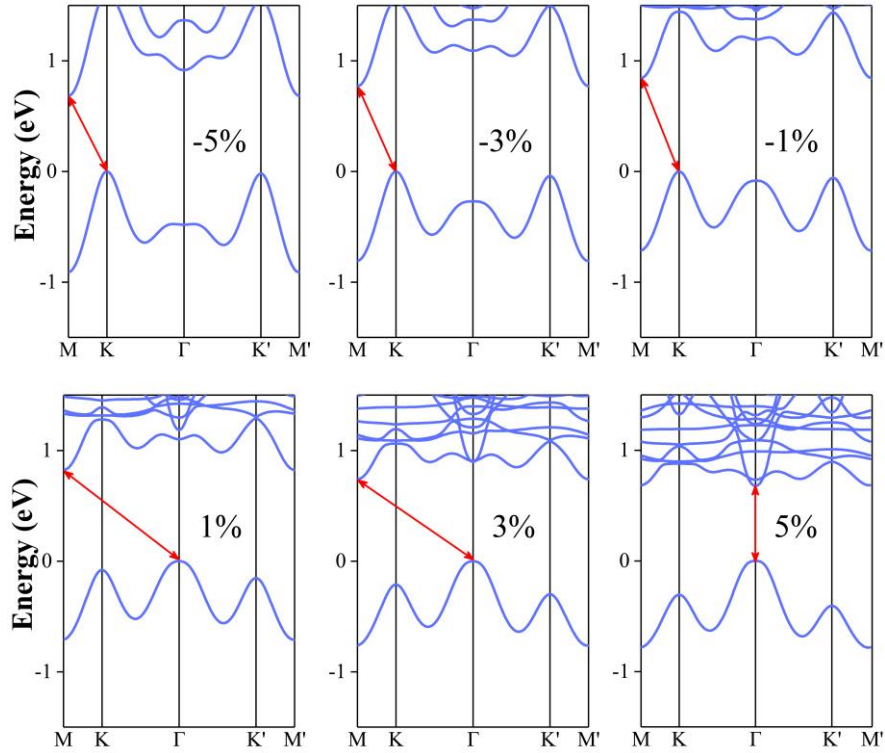

Fig. S7. Band structure of the monolayer GdClBr with SOC at different biaxial strains from -5% to 5%. Magnetic moments direction is along the z-aixs, and the Fermi level is set at VBM. The red arrows indicate the minimun band gaps.
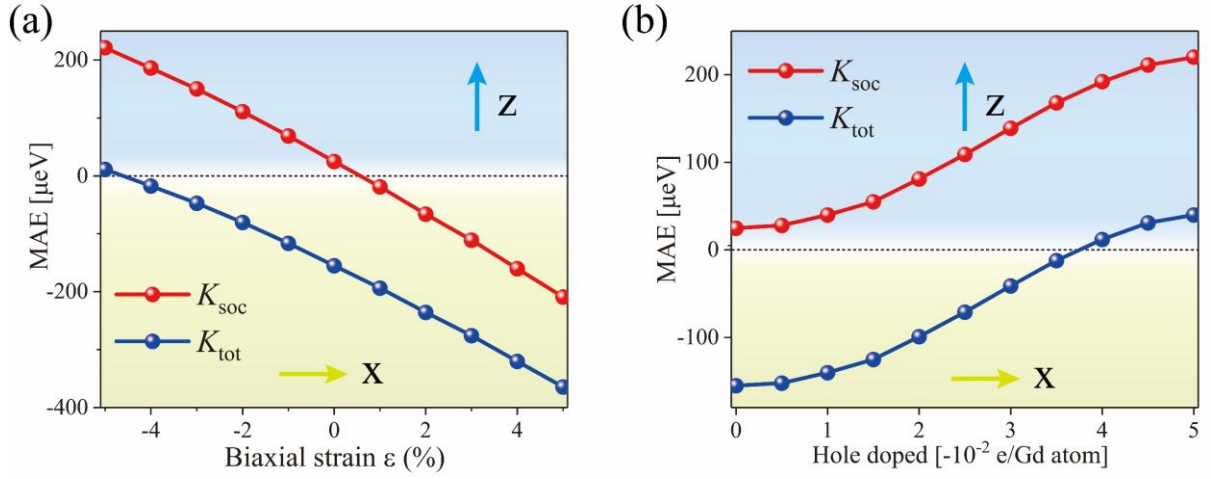
Fig. S8. The MAE of monolayer GdClBr varies with IP biaxial strain (a) and hole doping (b). The K_{SOC} is the single ion anisotropy arising from SOC and K_{tot} is the total single ion anisotropy containing K_{SOC} and K_{MDD} in our manuscript.
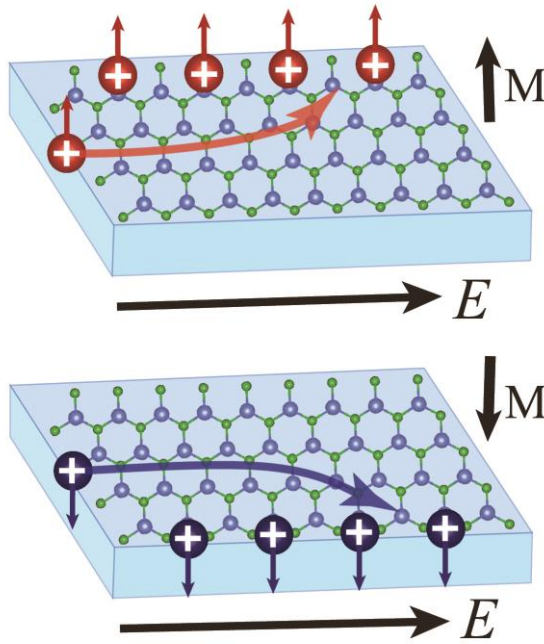

Fig. S9. The schematic diagram of the anomalous valley Hall effect (AVHE) of monolayer Gd*XY*.

The black arrows denote the orientations of magnetic moments and electric field.
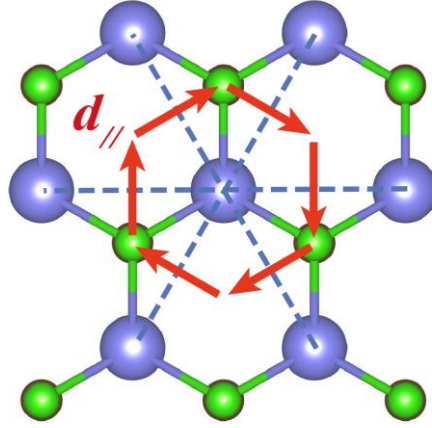
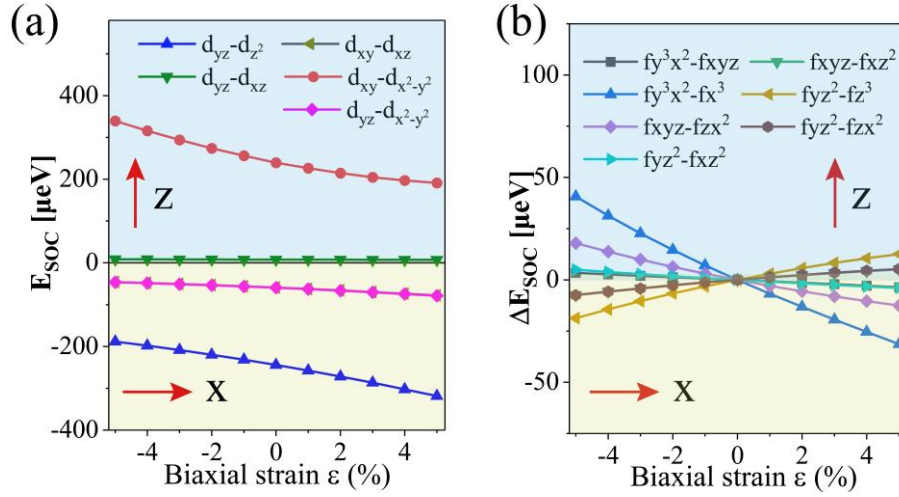**Fig. S10**. The in-plane DMI $d_{//}$ of monolayer GdXY.

Fig. S11. The contribution of d-orbital coupling matrix elements of monolayer GdClBr to the K_{SOC} as a function of biaxial strain (a). The contribution of f-orbital coupling matrix elements of monolayer GdClBr to the K_{SOC} with biaxial strain compared to without strain (b).

TABLE S1. The number of electrons gained by the X (Y) atom, e_X (e_Y) in units of e/atom, during the formation of the Gd-X(Y) bond, and the difference between e_X and e_Y, Δe_{X-Y} in units of e/atom.

	GdClBr	GdBrI	GdClI

e_X	0.734	0.707	0.7595
e_Y	0.677	0.638	0.6225
Δe_{X-Y}	0.057	0.069	0.137

TABLE S2. The elastic constants C_{11}/C_{12} (N/m) of monolayer GdClBr with biaxial strain of -5% (a), 0(b) and 5% (c).

	-5%	0	5%
C_{11}	61.98	44.18	31.89
C_{12}	16.20	13.34	11.32