Electronic Supplementary Information for

Dirac semimetallic Janus Ni-trihalide monolayer with strain-tunable magnetic anisotropy and electronic properties

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A. Bader analysis

Bader charge analysis is calculated to quantity the charge transfer in $Ni_2X_3Y_3$ (*X,Y*=I, Br, Cl; *X*≠*Y*) monolayers, as shown in Table S1.

Table S1 The charge transfer of each atom of $Ni_2X_3Y_3$ (*X,Y*=I, Br, Cl; *X*≠*Y*) monolayers.

	Δq_{Ni1}(e)	Δq_{Ni2}(e)	Δq_{X1}(e)	Δq_{X2}(e)	Δq_{X3}(e)	Δq_{Y1}(e)	Δq_{Y2}(e)	Δq_{Y3}(e)
$Ni_2Cl_3Br_3$	0.1203	0.1053	0.075	0.0864	0.0697	-0.0796	-0.1936	-0.2437
$Ni_2Cl_3I_3$	0.2804	0.2516	0.1443	0.1719	0.1405	-0.2185	-0.3888	-0.3816
$Ni_2Br_3I_3$	0.3844	0.3639	0.0292	0.0523	0.0294	-0.2022	-0.335	-0.3222

B. Band structure of $Ni_2X_3Y_3$ after applying SOC

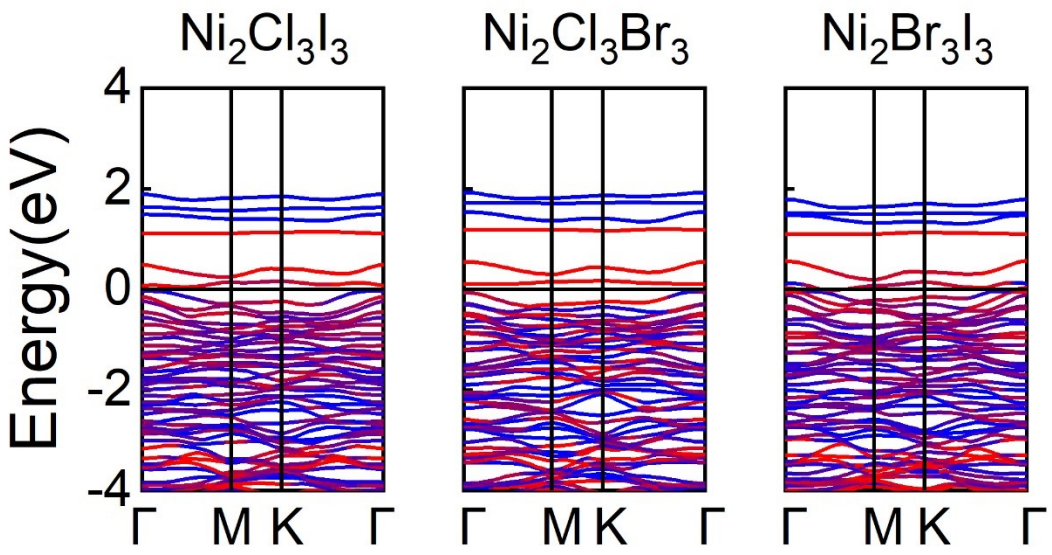

Fig. S1. The band structure of $Ni_2X_3Y_3$ using the PBE+*U*+SOC.

C. Density of states of $Ni_2Cl_3I_3$ and $Ni_2Cl_3I_3$ after applying in-plane biaxial strain

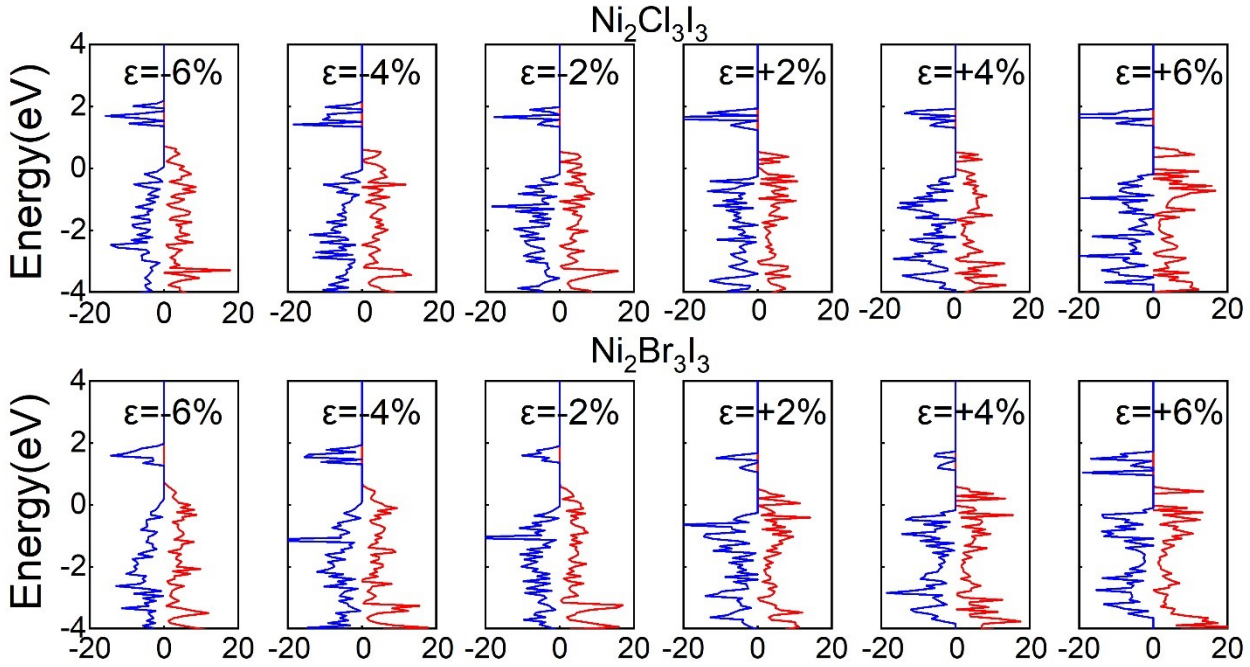

Fig. S2. The density of states of $Ni_2Br_3I_3$ and $Ni_2Br_3I_3$ after applying -6%, -4%, -2%, +2%, +4%, +6% in-plane biaxial strain.

D. Charge density difference and the planar average of electrostatic potential after applying in-plane biaxial strain

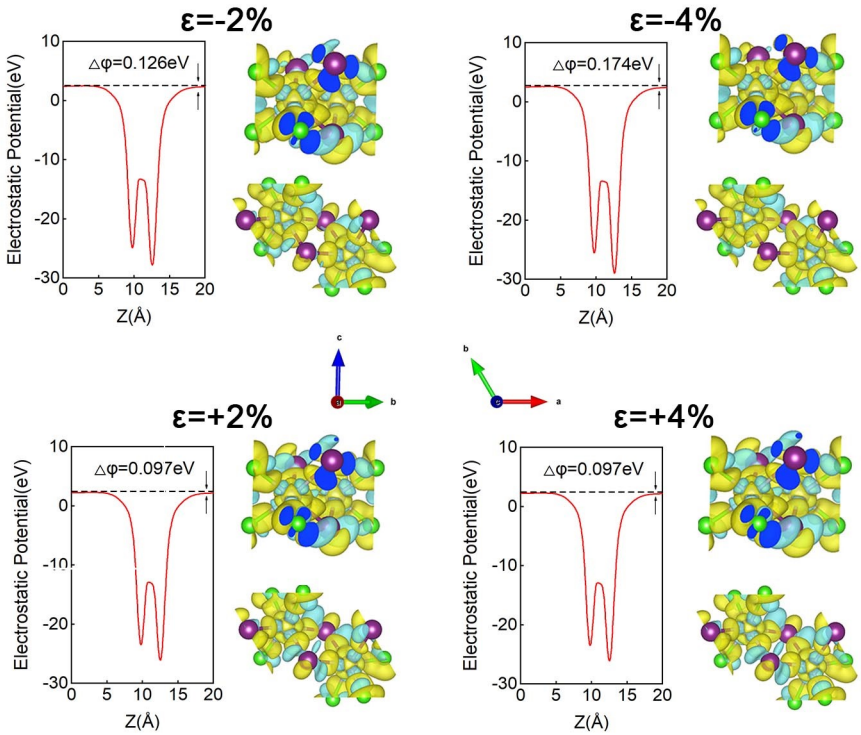

Fig. S3. Charge density difference of $Ni_2Cl_3I_3$ after applying -4%, -2%, +2%, +4%, in-plane biaxial strain, where yellow and blue regions represent the charge gain and loss. The planar average of electrostatic potential of $Ni_2Cl_3I_3$ after applying -4%, -2%, +2%, +4%, in-plane biaxial strain.

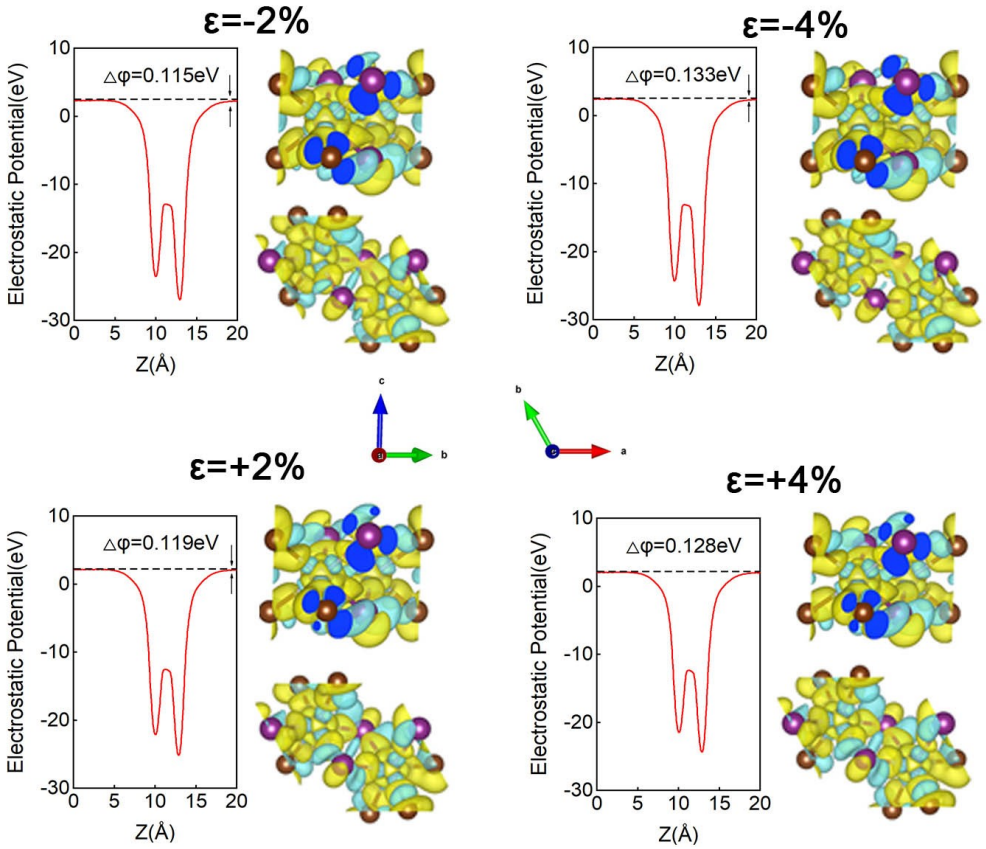

Fig. S4. Charge density difference after applying -4%, -2%, +2%, +4%, in-plane biaxial strain of $Ni_2Br_3I_3$, where yellow and blue regions represent the charge gain and loss. The planar average of electrostatic potential of $Ni_2Br_3I_3$ after applying -4%, -2%, +2%, +4%, in-plane biaxial strain.