Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Strain-tunable magnetic anisotropy in two-dimensional Dirac half-metals: Nickel Trihalides

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Table S1. Calculated lattice constants, Ni-X bond length l, Ni-X-Ni bond angle θ_1, X-Ni-X axial angle θ_2, cohesive energy E_{coh}, and 2D Young's modulus for the FM phase of the nickel trihalides. The energy difference between FM and various AFM states (E_{FM}–E_{AFM}) of the 2×2×1 supercell, magnetic moment of Ni ion, and MAE.

	Structural parameters					
	a (Å)	l (Å)	θ_1 (deg)	θ_2 (deg)	E_{coh} (eV/atom)	Y_{2D} (N m^{-1})
$NiCl_3$	5.940	2.296	96.6	171.9	–3.03	20.45
$NiBr_3$	6.313	2.452	96.0	171.6	–2.54	16.46
NiI_3	6.815	2.652	95.8	171.2	–1.98	10.41
	Magnetic parameters					
	$\Delta E_{Néel}$ (meV)	ΔE_{zigzag}	ΔE_{stripy}	ΔE_{mixed}	Mag_{Ni} (μ_B)	MAE (μeV/Ni)
$NiCl_3$	–537	–129	–327	–340	1.15	217.5
$NiBr_3$	–569	–155	–359	–368	1.18	263.5
NiI_3	–624	–178	–382	–391	1.23	-320.6

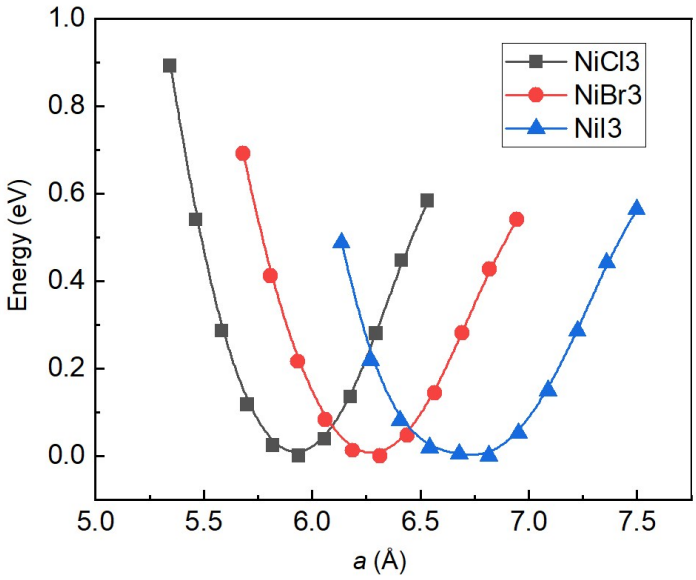

Fig. S1. Variation of relative energy with the 2D lattice constant for the monolayer NiX_3.

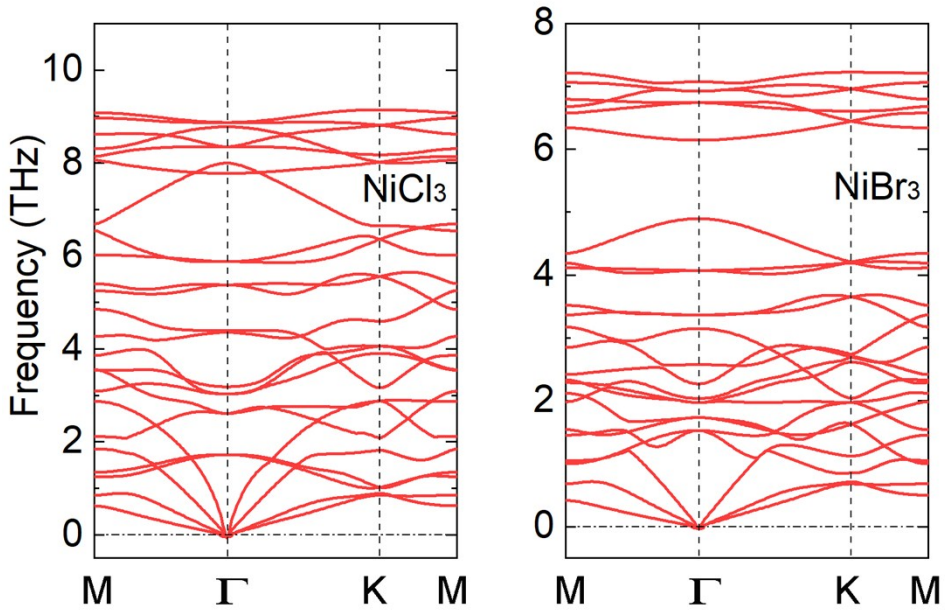

Fig. S2. Phonon bands of monolayer $NiCl_3$ and $NiBr_3$.

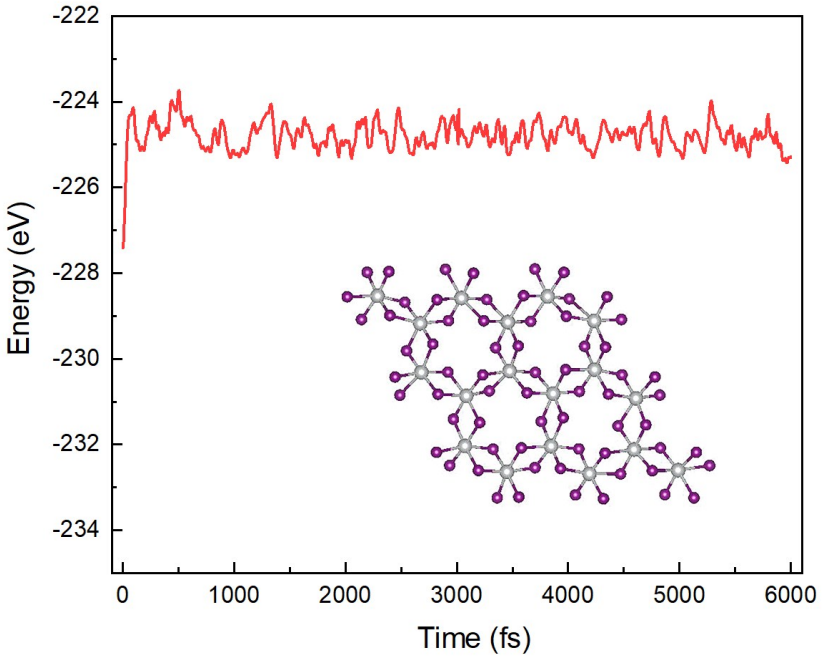

Fig. S3. Potential energy fluctuations of NiI_3 as a function of simulation time at 500 K. The inset shows the corresponding structure at 500 K after the simulation for 6 ps.

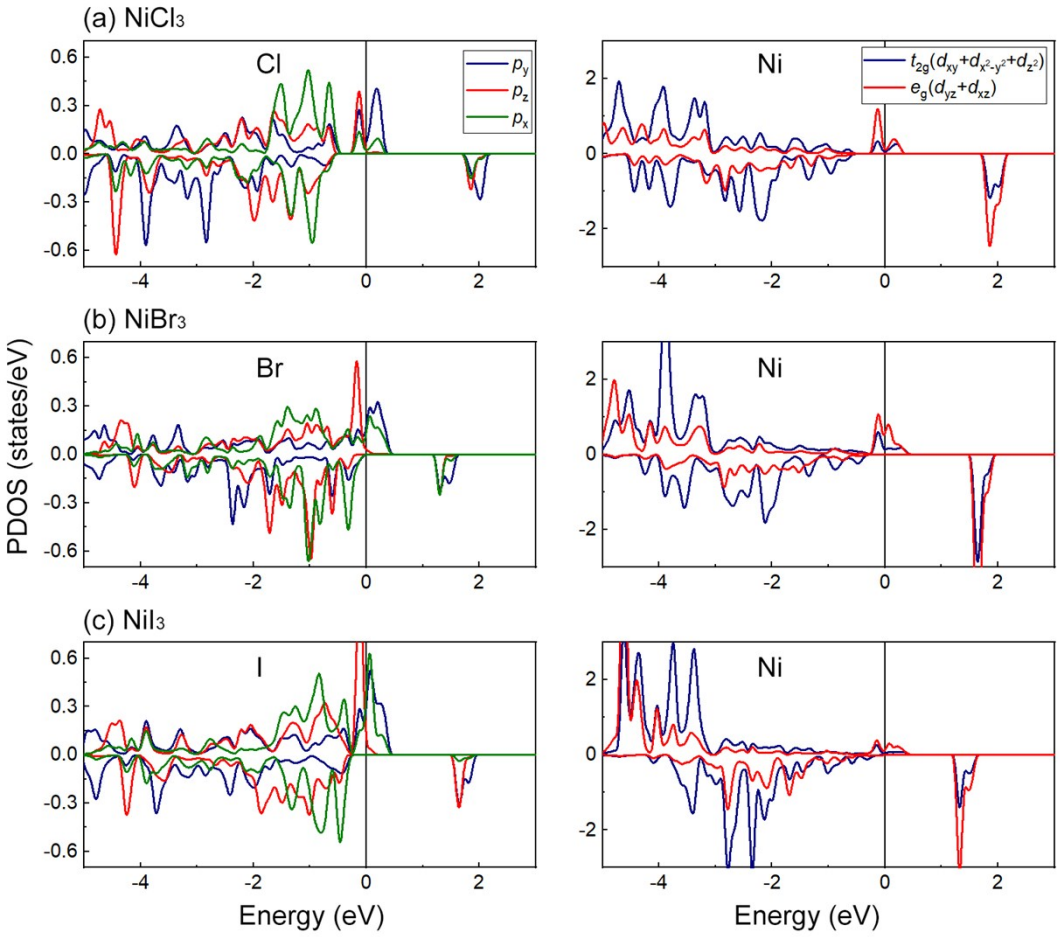

Fig. S4. PDOS of *p* orbitals for halogen atom and *d* orbitals for Ni atom in (a) $NiCl_3$, (b) $NiBr_3$, and (c) NiI_3 monolayer. The Fermi level is set to zero.

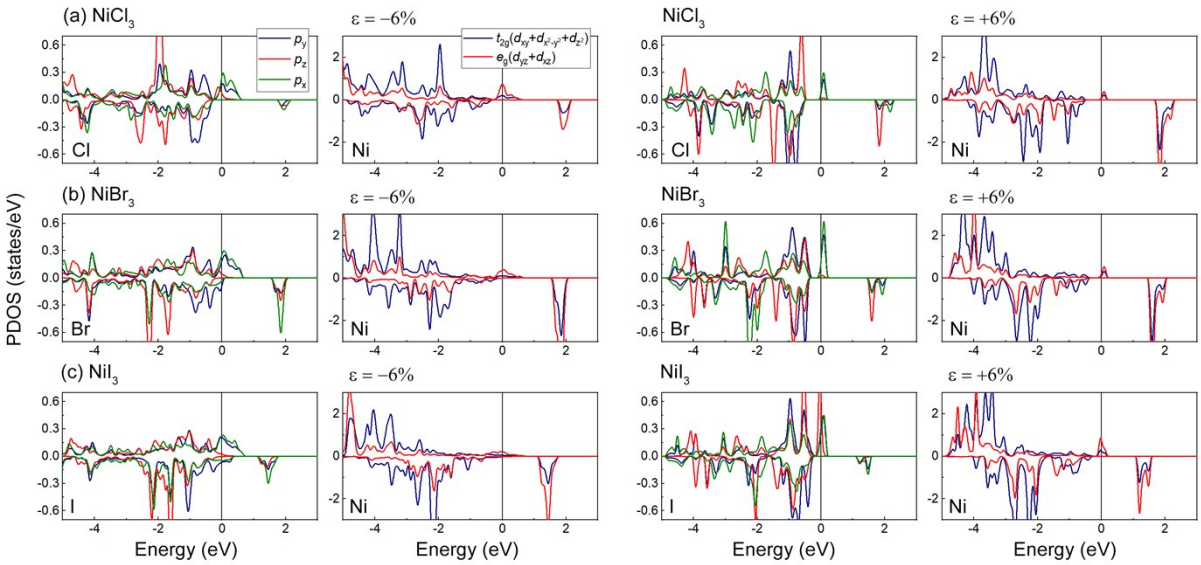

Fig. S5. PDOS of *p* orbitals for halogen atom and *d* orbitals for Ni atom in (a) $NiCl_3$, (b) $NiBr_3$, and (c) NiI_3 monolayer with the biaxial strain ε of –6% and +6%.