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Supplementary Information for "Doping-induced magnetism and magnetoelectric coupling in one-dimensional $NbOCl_3$ and $NbOBr_3$"

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Table S1. Total magnetic moments of different elements in the top and bottom cell as well as their moment differences for n-L nanochain of $NbOCl_3$, electing the doping concentration of $2.9\times10^{14}/cm^2$ and $\Delta\mu = \mu_{top} - \mu_{bot}$.

	2-L	3-L	4-L	5-L	6-L
Nb_{top}	0.696	0.806	0.95	1.006	1.036
Nb_{bot}	0.242	0.294	0.304	0.344	0.354
$\Delta\mu_{Nb}$	0.454	0.512	0.646	0.662	0.682
Cl_{top}	0.074	0.072	0.09	0.09	0.09
Cl_{bot}	0.008	0.014	0.004	0.006	0.006
$\Delta\mu_{Cl}$	0.066	0.058	0.086	0.084	0.084
O_{top}	-0.032	-0.04	-0.044	-0.048	-0.05
O_{bot}	-0.016	-0.018	-0.022	-0.024	-0.024
$\Delta\mu_{O}$	-0.016	-0.022	-0.022	-0.024	-0.026

Table S2. Total magnetic moments of different elements in the top and bottom cell as well as their moment differences for n-L nanochain of $NbOBr_3$, electing the doping concentration of $2.9\times10^{14}/cm^2$ and $\Delta\mu = \mu_{top} - \mu_{bot}$.

	2-L	3-L	4-L	5-L	6-L
Nb_{top}	0.76	0.794	1.068	1.04	1.11
Nb_{bot}	0.264	0.29	0.232	0.288	0.326
$\Delta\mu_{Nb}$	0.496	0.504	0.836	0.752	0.784
Br_{top}	0.034	0.024	0.098	0.098	0.099
Br_{bot}	0.01	0.014	-0.008	0	0.002
$\Delta\mu_{Br}$	0.024	0.01	0.106	0.098	0.097
O_{top}	-0.048	-0.054	-0.052	-0.052	-0.056
O_{bot}	-0.016	-0.016	-0.02	-0.02	-0.024
$\Delta\mu_{O}$	-0.032	-0.038	-0.032	-0.032	-0.032

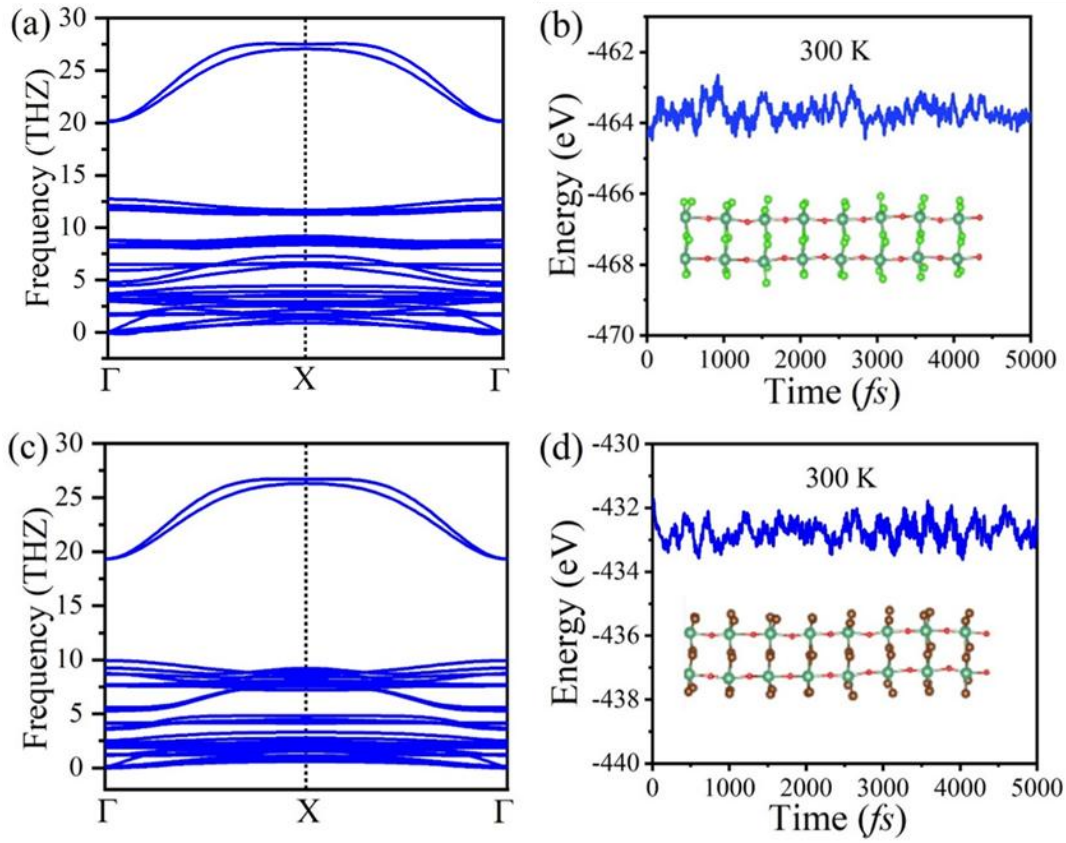

Figure S1. The phonon spectra of (a) 1D $NbOCl_3$ and (c) 1D $NbOBr_3$. The evolutions of the total energy of (b) 1D $NbOCl_3$ and (d) 1D $NbOBr_3$ with time at 300K through the AIMD simulations, and illustrations are the final atomic structures.

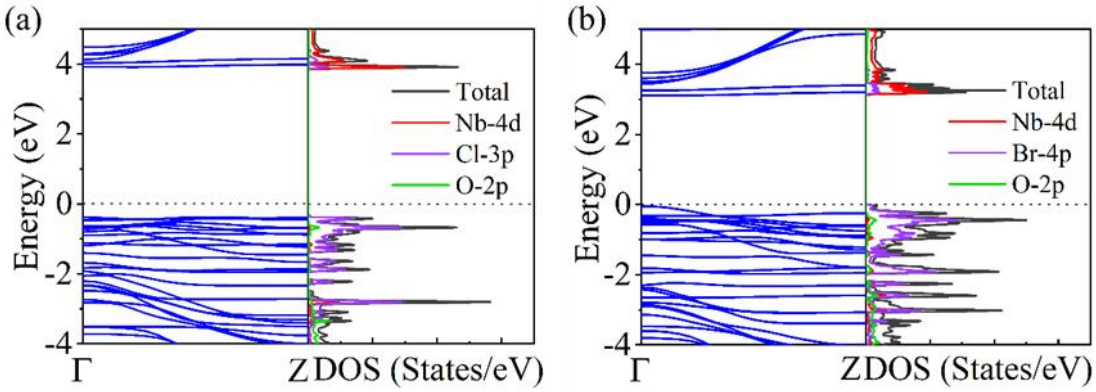

Figure S2. The band structures and projected densities of orbital states of (a) 1D $NbOCl_3$ and (b) 1D $NbOBr_3$ calculated by HSE method.

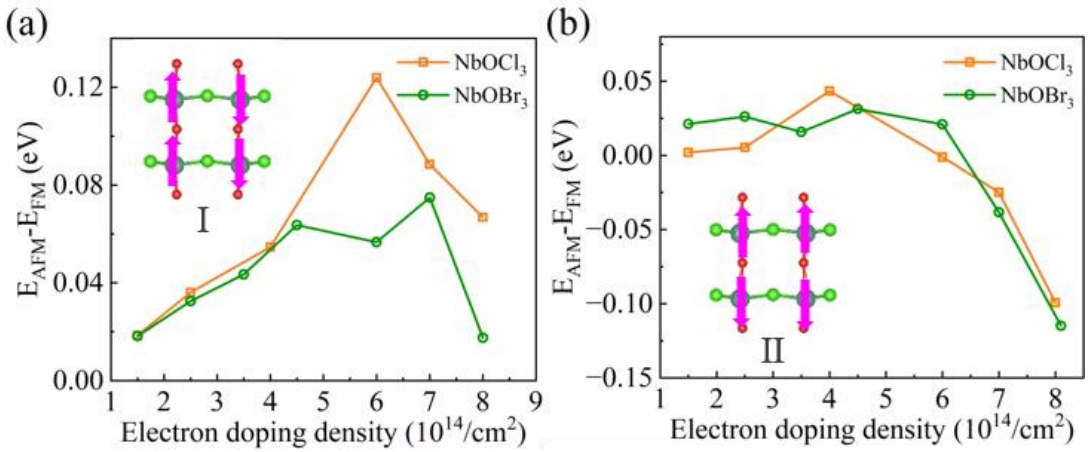

Figure S3. (a) and (b) are the energy difference of FM and two types of AFM ($\Delta E = E_{AFM} - E_{FM}$) as a function of the electron-doping concentration in 1D $NbOX_3$ (X=Cl, Br), the illustrations are the corresponding schematic diagrams of two types of antiferromagnetic orders.

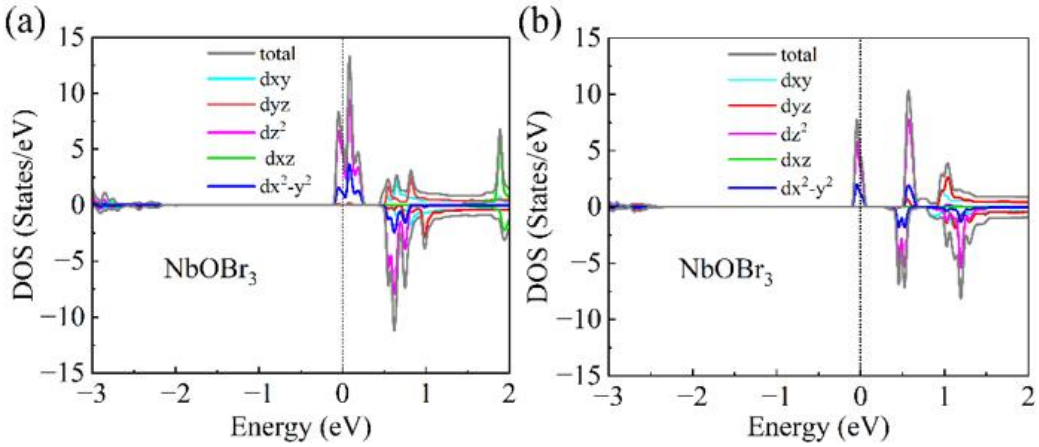

Figure S4. The PDOS of Nb-d orbital for (a) 1D $NbOCl_3$ at the concentration of $4.0\times10^{14}/cm^2$ and (b) 1D $NbOBr_3$ at the concentration of $3.9\times10^{14}/cm^2$.

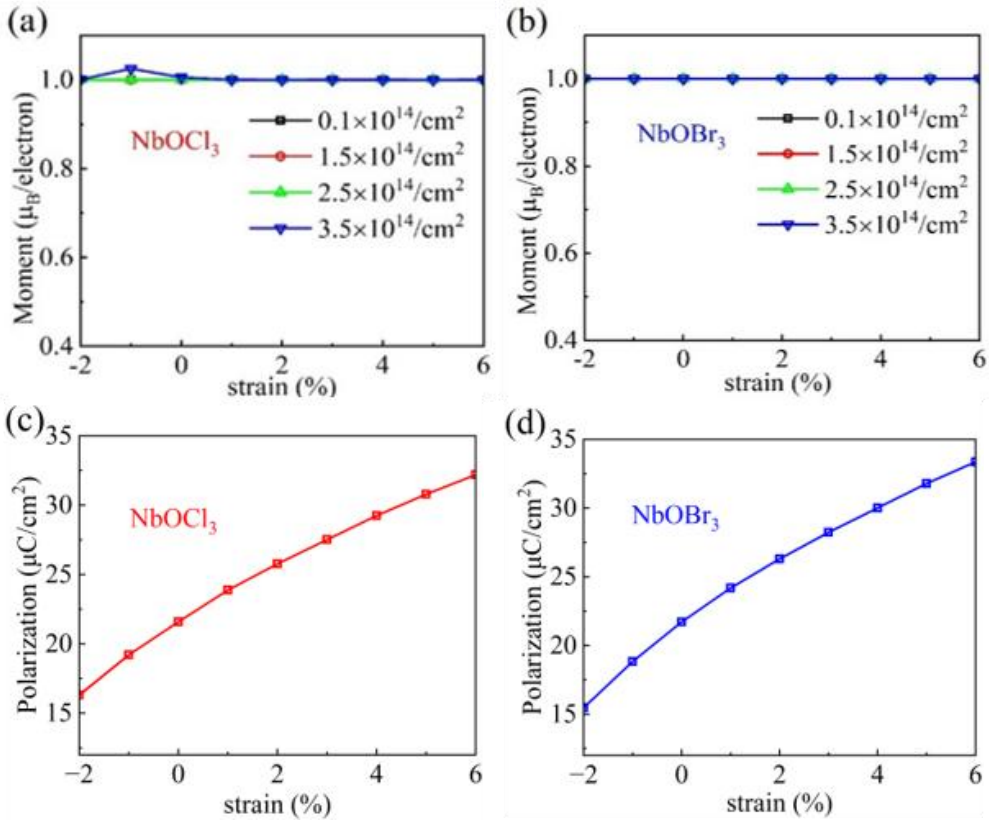

Figure S5. The doping-induced magnetic moment vs strain in (a) 1D $NbOCl_3$ and (b) 1D $NbOBr_3$ at different doping-electrons concentrations. The ferroelectric polarization under different strains without doping in (c) 1D $NbOCl_3$ and (d) 1D $NbOBr_3$.

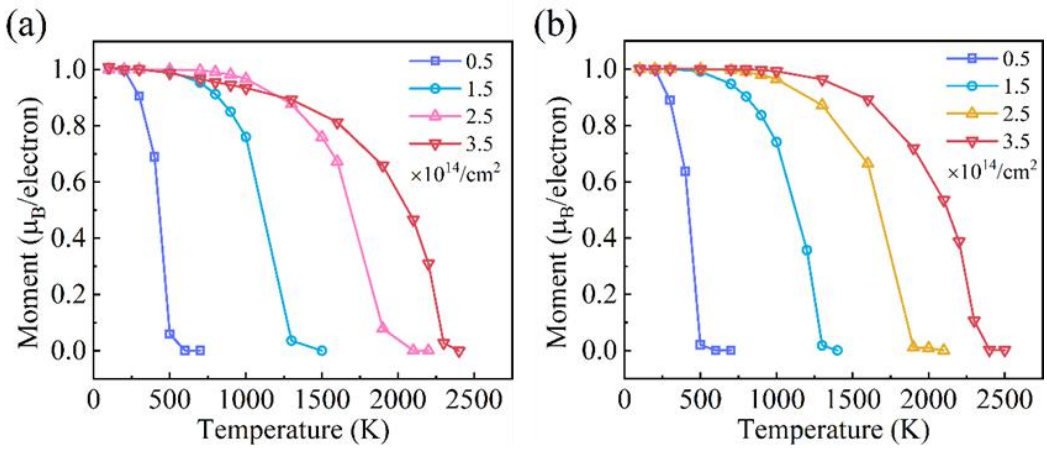

Figure S6. The spin magnetic moment vs temperature for (a) 1D $NbOCl_3$ and (b) 1D $NbOBr_3$ at different doping concentrations. In this simulation, the magnetic carriers are approximated to satisfy the Fermi-Dirac distribution function $f\left(\frac{\varepsilon-\mu}{\sigma}\right)=\frac{1}{exp\left(\frac{\varepsilon-\mu}{\sigma}+1\right)}$, where μ is the chemical potential, and $\sigma = \kappa_B T$ is the energy broadening factor that introduces temperature effect.

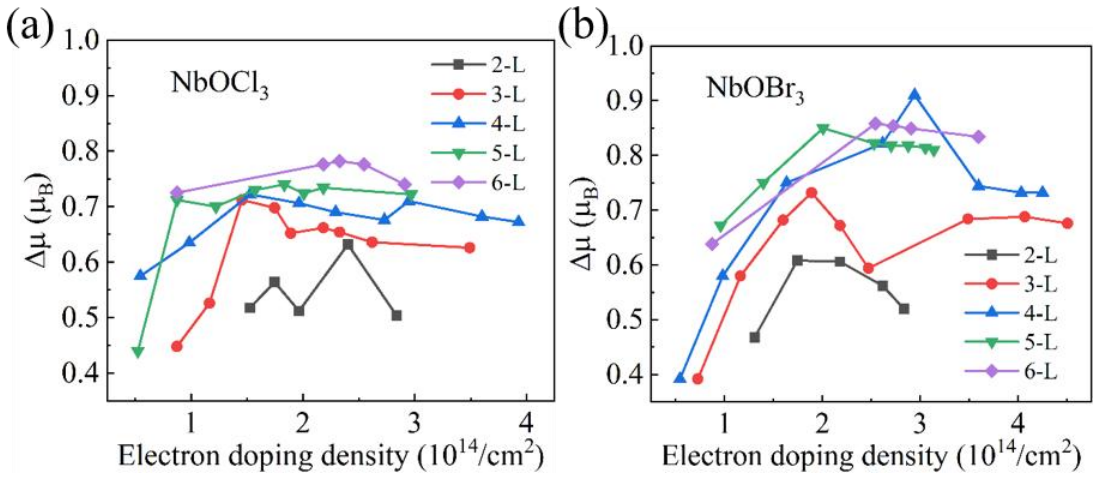

Figure S7. The magnetic moment difference ($\Delta\mu = \mu_{top} - \mu_{bot}$) of (a) n-L $NbOCl_3$ and (b) n-L $NbOBr_3$ nanochains under different doping concentrations.

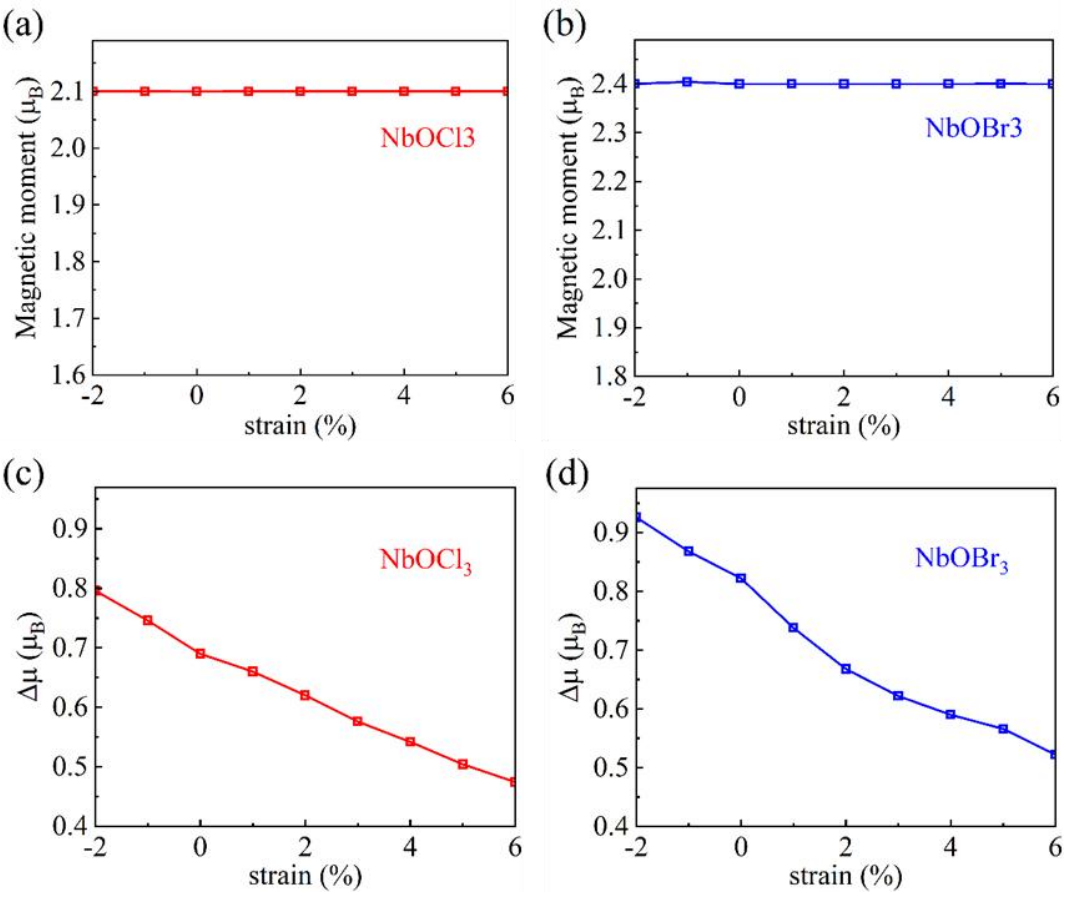

Figure S8. Under different strains, (a) the total magnetic moments and (b) magnetic moment differences of 4-L $NbOCl_3$ at the concentration of $2.29\times10^{14}/cm^2$ (doping about 2.1 electrons), (a) the total magnetic moments and (b) magnetic moment differences of 4-L $NbOBr_3$ at the concentration of $2.62\times10^{14}/cm^2$ (doping about 2.4 electrons).