Supporting Information:

Preparation and multiferroicity of a novel two-dimensional material NiH_2SeO_4

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Fig. S1 Thermogravimetric and differential scanning calorimetry (TGA/DSC) vs. temperature for NiH_2SeO_4.

Fig. S2 NiH_2SeO_4 Powder XRD after heating at 200 °C.

Fig. S3 Schematic diagram of polarization caused by selenium distortion

Fig. S4 The electronic image of NiH_2SeO_4 and the EDS energy spectrum of the corresponding selection.

Fig. S5 Absorption spectra of NiH_2SeO_4 polycrystalline samples converted from diffusion reflectance using the K–M function. The inset is its band gap fit.

Fig. S6 The Curie temperature of monolayer NiH_2SeO_4 though Monte Carlo (MC) simulations based on Ising model.

Fig. S7 The contact angle measured by water droplets on NiH_2SeO_4 film.

Table 1 Magnetic anisotropy of NiH_2SeO_4 monolayer. The energy in unit of μeV per Ni is referenced to the (1 0 0) direction.

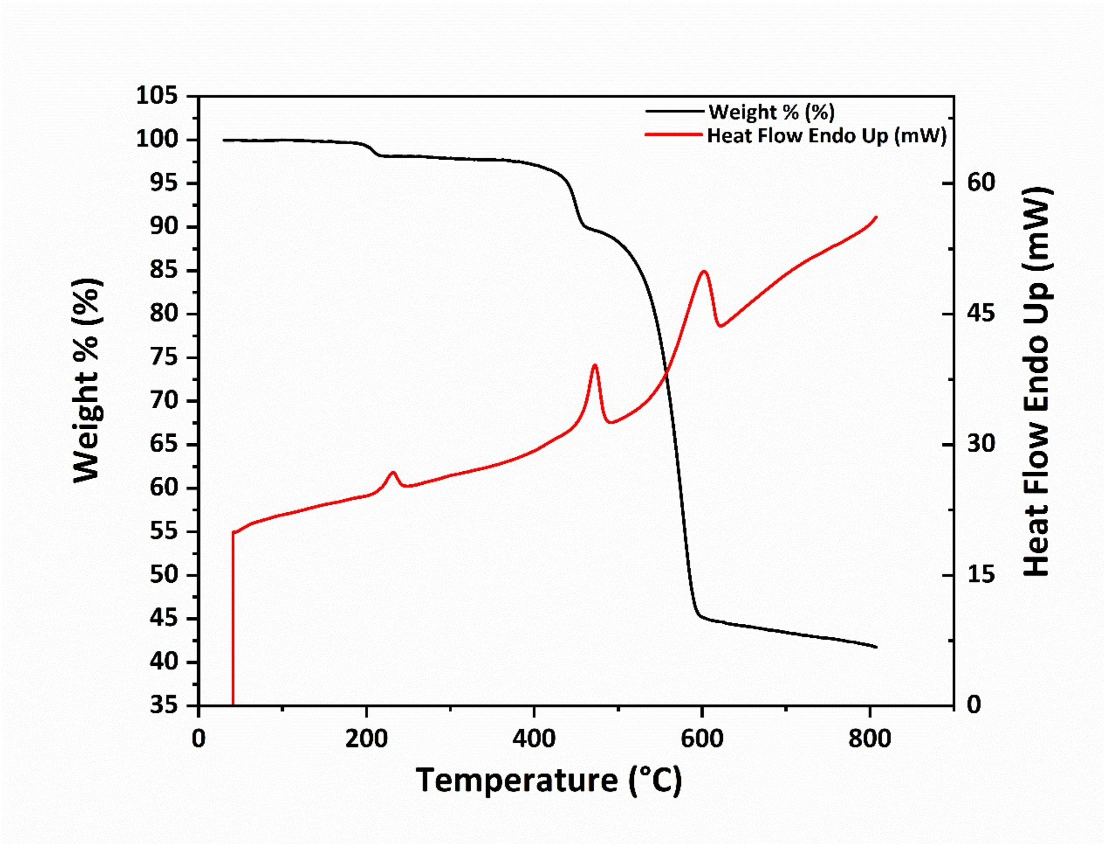

Fig. S1 Thermogravimetric and differential scanning calorimetry (TGA/DSC) vs. temperature for NiH_2SeO_4

Thermogravimetric analysis and differential scanning calorimetry analysis were performed to evaluate the thermal stability of NiH_2SeO_4. As shown in the TGA/DSC curve (Fig. S1), the compound is stable from room temperature to 200°C in a nitrogen atmosphere. From 200°C to 451°C, the mass loss is 8.4%, accompanied by an endothermic peak. This means that H_2O is released from the structure (calculated value: 8.8%). The next decomposition process is from 451°C to 581°C, and the total mass loss is approximately 47% (calculated value: 46.6%), which corresponds to the dissociation of SeO_2 from the structure.

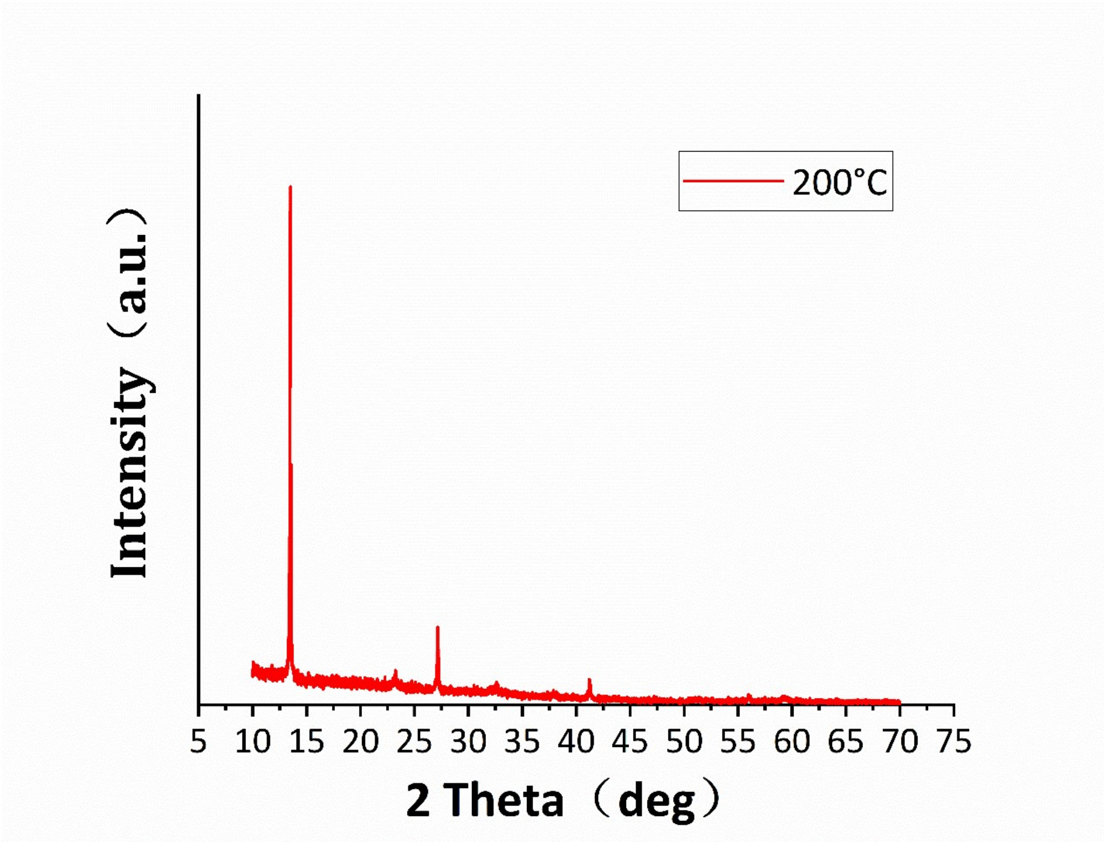

Fig. S2 NiH_2SeO_4 Powder XRD after heating at 200°C.

The peak at 200°C may be caused by the absorption of water molecules. After taking a certain sample and heating for 4 hours at 200°C, the powder XRD pattern was collected, and the XRD peak did not shift, which means that the structural H_2O did not release.

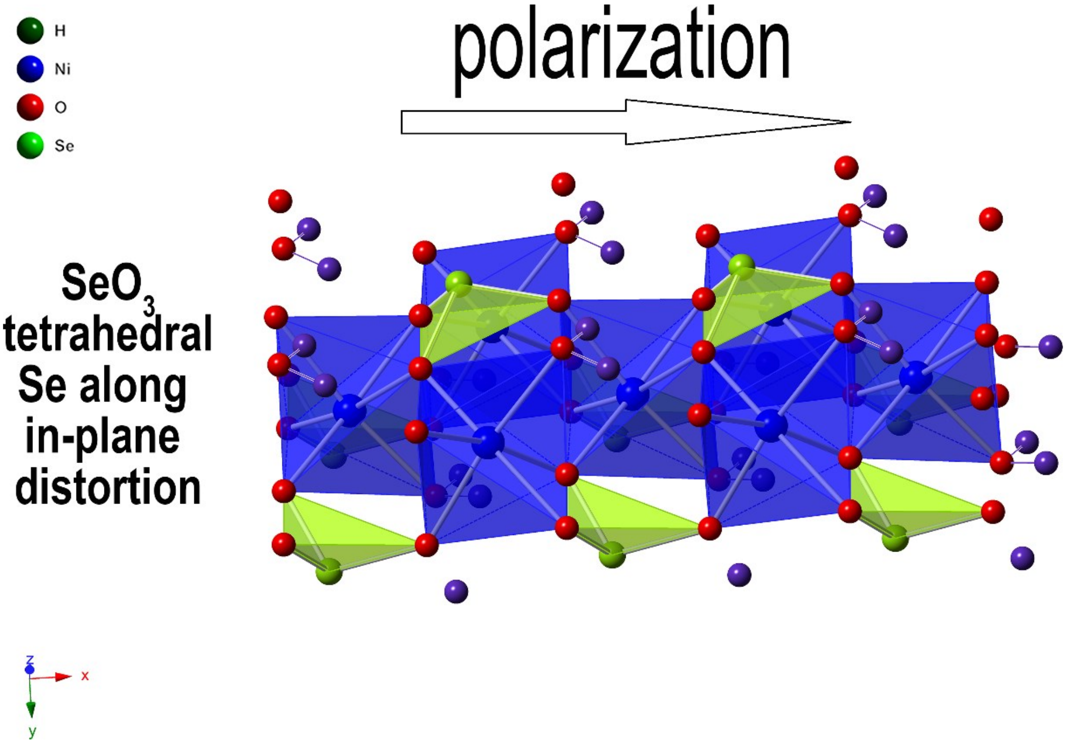

Fig. S3 Schematic diagram of polarization caused by selenium distortion

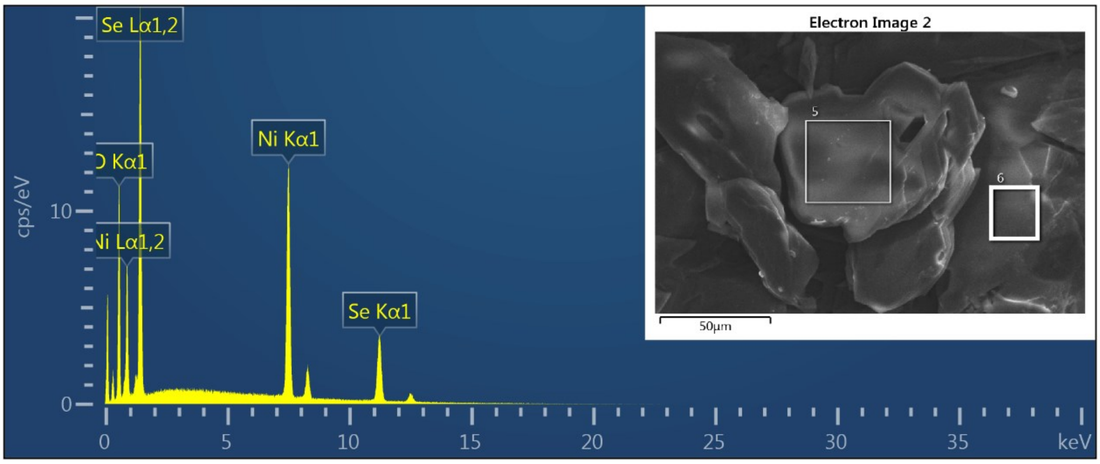

Fig. S4 The scanning electron miscroscopy (SEM) image of NiH_2SeO_4 crystal and the electron dispersive spectroscopy (EDS) spectrum of the corresponding selection.

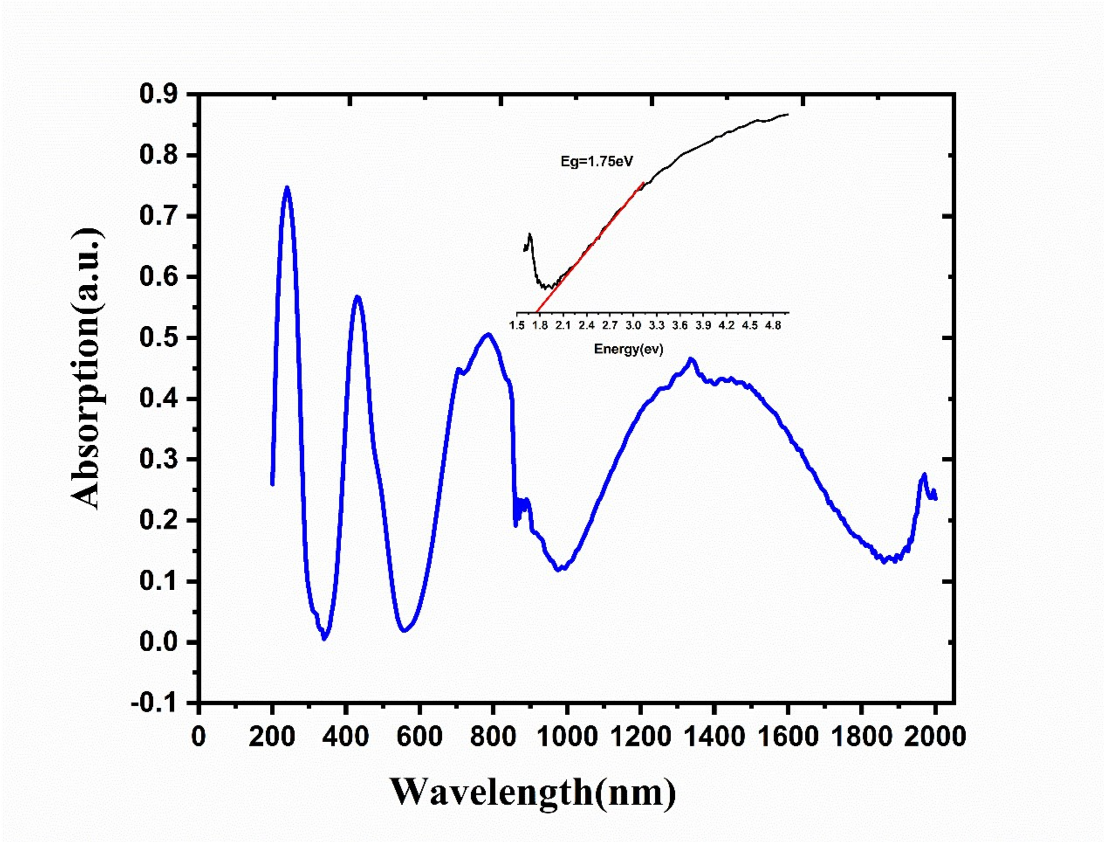

Fig. S5 Absorption spectra of NiH_2SeO_4 powder samples converted from diffusion reflectance using the K–M function. The inset is the fitting for obtaining band gap, which is approximately 1.75 ev.

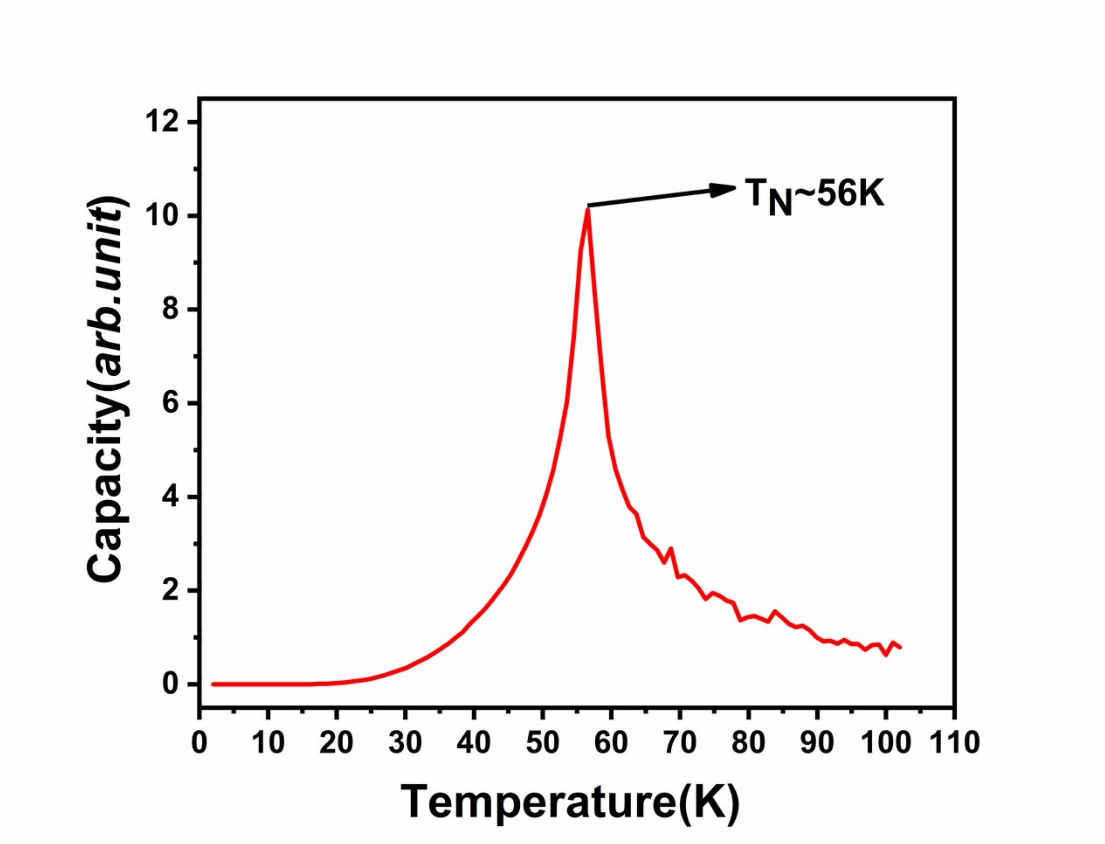

Fig. S6 The Curie temperature of monolayer NiH_2SeO_4 though Monte Carlo (MC) simulations based on Ising model

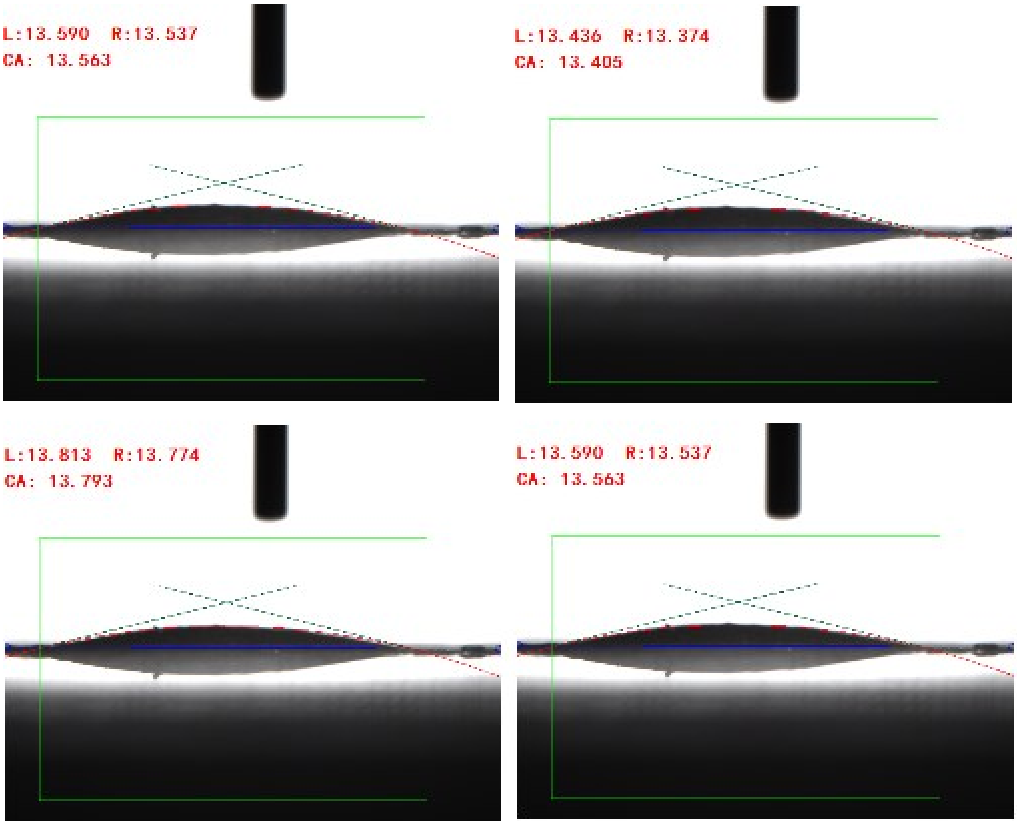

Fig. S7 The contact angle measured by water droplets on NiH_2SeO_4 film.

Fig. S7 shows the water drop angle measurement of sample films coated on the PET film by spin coating. The size of the contact angle reflects the hydrophilicity of the membrane, showing good hydrophilicity.

Table S1 Magnetic anisotropy of NiH_2SeO_4 monolayer. The energy in unit of μeV per Ni is referenced to the (1 0 0) direction.

0 1 0	0 0 1	1 1 -1	1 -1 1	-1 1 1	1 -1 -1	-1 1 -1	-1 -1 1	1 1 1	1 1 0	1 0 1	0 1 1
312	403	133	233	356	133	215	356	233	139	190	379