Supporting Information:

Preparation and multiferroicity of a novel two-dimensional material NiH$_2$SeO$_4$

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**Fig. S1** Thermogravimetric and differential scanning calorimetry (TGA/DSC) vs. temperature for NiH$_2$SeO$_4$.

**Fig. S2** NiH$_2$SeO$_4$ Powder XRD after heating at 200 °C.

**Fig. S3** Schematic diagram of polarization caused by selenium distortion.

**Fig. S4** The electronic image of NiH$_2$SeO$_4$ and the EDS energy spectrum of the corresponding selection.

**Fig. S5** Absorption spectra of NiH$_2$SeO$_4$ 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$_2$SeO$_4$ though Monte Carlo (MC) simulations based on Ising model.

**Fig. S7** The contact angle measured by water droplets on NiH$_2$SeO$_4$ film.

**Table 1** Magnetic anisotropy of NiH$_2$SeO$_4$ monolayer. The energy in unit of μeV per Ni is referenced to the (1 0 0) direction.
Thermogravimetric and differential scanning calorimetry (TGA/DSC) analysis were performed to evaluate the thermal stability of NiH$_2$SeO$_4$. 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$_2$O 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$_2$SeO$_4$ 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$_2$O did not release.
Fig. S3 Schematic diagram of polarization caused by selenium distortion
Fig. S4 The scanning electron microscopy (SEM) image of NiH$_2$SeO$_4$ crystal and the electron dispersive spectroscopy (EDS) spectrum of the corresponding selection.
**Fig. S5** Absorption spectra of NiH$_2$SeO$_4$ powder samples converted from diffusion reflectance using the K–M function. The inset is the fitting for obtaining band gap, which is approximately $1.75 \text{ ev}$. 
Fig. S6  The Curie temperature of monolayer NiH$_2$SeO$_4$ though Monte Carlo (MC) simulations based on Ising model
Fig. S7 The contact angle measured by water droplets on NiH$_2$SeO$_4$ 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>
<thead>
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<th>Table S1</th>
<th>Magnetic anisotropy of NiH$_2$SeO$_4$ monolayer. The energy in unit of µeV per Ni is referenced to the (1 0 0) direction.</th>
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