Supplementary Information (SI) for Nanoscale.
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Regulating magnetic skyrmions in multiferroic monolayer MnOBr

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Machine learning method

In the input data of this paper, there are 20,000 atoms per image and each atom has three spin directions. The total number of data dimensions reaches 60,000. The first thing we need to do is to reduce the input data dimensions. The identification of spin textures can be considered as image recognition and we can use an image dimensionality reduction algorithm on it. Scale Invariant Feature Transform (SIFT)[1] is an image localized feature extraction algorithm and can be used for image dimensionality reduction. It extracts features by finding the precise location of extreme points and constructing key point descriptors.

First, SIFT uses the Gaussian kernel for image smoothing: The original image is performed as the first interval and Gaussian convolution is performed on it to get the second interval. The Gaussian convolution function is:

$$G(x,y) = \frac{1}{2\pi\sigma^2} e^{-\frac{(x-x_0)^2+(y-y_0)^2}{2\sigma^2}}, \tag{1}$$

where σ is a fixed value of 1.6. Then, Multiplying σ by a scaling factor k, we obtains a new smoothing factor $\sigma = k \cdot \sigma$. It is used to convolve the second interval to get the third Interval. We repeat this and so on to end up with L interval. In this way, we get the first octave of images. The penultimate third interval image of octave 1 is downsampled with a scale factor of 2, and the image obtained is used as the first interval of octave 2. This is repeated to get a total of O octaves with L intervals each, totaling $O \cdot L$ images. In this work, $k = 2^{1/7}$, $L = 10$ and $O = 6$. And the images are differenced to get the feature points. Finally, the region is divided into 4×4 sub-blocks, and feature point counting operations are performed in 8 directions for each sub-block to obtain the gradient magnitude in each direction, which can form a total of 128-dimensional description vectors. In this way, we reduce 30,000 dimensions of input data to 128 dimensions.

After SIFT reduced the data dimensions, we use Gaussian Mixture Model (GMM)[2] to cluster the data. It relies on the model itself to cluster data with a high degree of similarity into one class instead of inputting classification labels. With this approach, we minimize human subjective influence in the classification. We use the python library sklearn[3] for the GMM implementation. In the GMM, there are four hyperparameters: number of clusters (k), maximum number of iterations (maxIter), random number seed (seed) and convergence threshold of the log-likelihood function (Tol). In this work, k = 4, maxlter = 150, seed is the default value, Tol = 0.05.

We use the clustering results of the GMM to fit the relationship between deformation and applied magnetic field with the spin textures using the Support Vector Machine (SVM).[4] Then, we drew the phase diagram with predictions of SVM. We use the python library sklearn for the SVM implementation. The hyperparameters of the SVM are: kernel function (kernel), standard deviation (gamma), penalty coefficient (C) and proportion of weight (class-weight). In this work, the kernel function is polynomial, gamma=2, C=800 and class-weight=balanced

Supplementary data for First-principle calculations

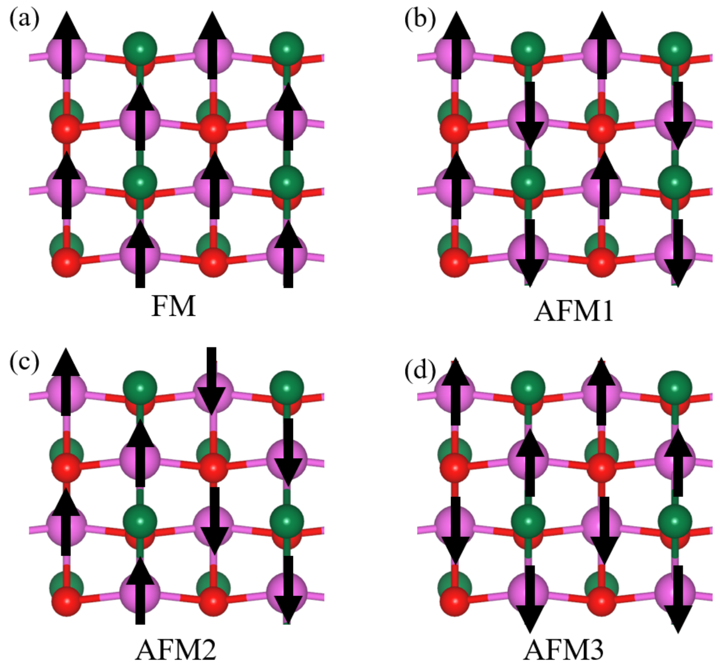

Figure S1: 4 magnetic orders of monolayer MnOBr: (a)FM, (b)AFM1, (c)AFM2, and (d)AFM3. Black arrows represent spin in different directions.

Table S1: Elastic constants of monolayer MnOBr (Gpa).

	C_{11}	C_{12}	C_{22}	C_{66}
MnOBr	43.0	19.5	65.1	17.9

References

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(3) F. Pedregosa, G. Varoquaux, A. Gramfort,V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss and V. Dubourg, *J. Mach. Learn. Res*, **2011**, *12*, 2825–2830.

(4) S. Suthaharan, *Integr. Ser. Inf. Syst*, **2016**, *36*, 1–12.