Moiré magnetic exchange interactions in twisted magnets

In addition to moiré superlattices, twisting can also generate moiré magnetic exchange interactions (MMEIs) in van der Waals magnets. However, owing to the extreme complexity and twist-angle-dependent sensitivity, all existing models fail to fully capture MMEIs and thus cannot provide an understanding of MMEI-induced physics. Here, we develop a microscopic moiré spin Hamiltonian that enables the effective description of MMEIs via a sliding-mapping approach in twisted magnets, as demonstrated in twisted bilayer CrI₃. We show that the emergence of MMEIs can create a magnetic skyrmion bubble with non-conserved helicity, a ‘moiré-type skyrmion bubble’. This represents a unique spin texture solely generated by MMEIs and ready to be detected under the current experimental conditions. Importantly, the size and population of skyrmion bubbles can be finely controlled by twist angle, a key step for skyrmion-based information storage. Furthermore, we reveal that MMEIs can be effectively manipulated by substrate-induced interfacial Dzyaloshinskii–Moriya interactions, modulating the twist-angle-dependent magnetic phase diagram, which solves outstanding disagreements between theories and experiments.

Moiré superlattices, which can host fascinating properties and support intriguing applications, can be constructed by stacking two van der Waals layered materials with a relatively small twist angle ($\theta$)\(^1\)\(^-\)\(^2\). Such a twist angle offers a new degree of freedom to effectively modulate fundamental electronic structures, providing an unconventional approach to generating and manipulating physical phenomena in various 2D van der Waals systems, for example, moiré flat bands\(^3\), unconventional superconductivity\(^4\),\(^5\), moiré Hubbard and Kane–Mele–Hubbard models\(^6\),\(^7\), and moiré excitons\(^8\),\(^9\). Importantly, developing effective theories to capture the electronic structures of extremely large-scale moiré lattices plays an indispensable role in understanding these interesting moiré-type phenomena\(^1\(^4\),\(^1\(^5\).\(^1\(^6\).\(^1\(^7\).\(^1\(^8\).\(^1\(^9\).\(^2\(^0\).\(^2\(^1\).\(^2\(^2\).\(^2\(^3\).\(^2\(^4\).\(^2\(^5\)\(^-\)\(^2\(^6\).\(^2\(^7\).\(^2\(^8\).\(^2\(^9\).\(^3\(^0\)\(^-\)\(^3\(^1\).\(^3\(^2\)\(^-\)\(^3\(^3\).\(^3\(^4\)\(^-\)\(^3\(^5\).\(^3\(^6\).\(^3\(^7\).\(^3\(^8\).\(^3\(^9\).\(^4\(^0\).\(^4\(^1\).\(^4\(^2\).\(^4\(^3\).\(^4\(^4\).\(^4\(^5\).\(^4\(^6\).\(^4\(^7\).\(^4\(^8\).\(^4\(^9\).\(^5\(^0\).\(^5\(^1\).\(^5\(^2\).\(^5\(^3\).\(^5\(^4\).\(^5\(^5\).\(^5\(^6\).\(^5\(^7\).\(^5\(^8\).\(^5\(^9\).\(^6\(^0\)\(^-\)\(^6\(^1\).\(^6\(^2\)\(^-\)\(^6\(^3\).\(^6\(^4\).\(^6\(^5\).\(^6\(^6\).\(^6\(^7\).\(^6\(^8\).\(^6\(^9\).\(^7\(^0\)\(^-\)\(^7\(^1\).\(^7\(^2\)\(^-\)\(^7\(^3\).\(^7\(^4\).\(^7\(^5\).\(^7\(^6\).\(^7\(^7\).\(^7\(^8\).\(^7\(^9\).\(^8\(^0\).\(^8\(^1\).\(^8\(^2\).\(^8\(^3\).\(^8\(^4\).\(^8\(^5\).\(^8\(^6\).\(^8\(^7\).\(^8\(^8\).\(^8\(^9\).\(^9\(^0\)\(^-\)\(^9\(^1\).\(^9\(^2\)\(^-\)\(^9\(^3\).\(^9\(^4\).\(^9\(^5\).\(^9\(^6\).\(^9\(^7\).\(^9\(^8\).\(^9\(^9\).\(^0\(^0\).\(^0\(^1\).\(^0\(^2\).\(^0\(^3\).\(^0\(^4\).\(^0\(^5\).\(^0\(^6\).\(^0\(^7\).\(^0\(^8\).\(^0\(^9\).\(^1\(^0\).\(^1\(^1\).\(^1\(^2\).\(^1\(^3\).\(^1\(^4\).\(^1\(^5\).\(^1\(^6\).\(^1\(^7\).\(^1\(^8\).\(^1\(^9\).\(^2\(^0\).\(^2\(^1\).\(^2\(^2\).\(^2\(^3\).\(^2\(^4\).\(^2\(^5\).\(^2\(^6\).\(^2\(^7\).\(^2\(^8\).\(^2\(^9\).\(^3\(^0\).\(^3\(^1\).\(^3\(^2\).\(^3\(^3\).\(^3\(^4\).\(^3\(^5\).\(^3\(^6\).\(^3\(^7\).\(^3\(^8\).\(^3\(^9\).\(^4\(^0\).\(^4\(^1\).\(^4\(^2\).\(^4\(^3\).\(^4\(^4\).\(^4\(^5\).\(^4\(^6\).\(^4\(^7\).\(^4\(^8\).\(^4\(^9\).\(^5\(^0\).\(^5\(^1\).\(^5\(^2\).\(^5\(^3\).\(^5\(^4\).\(^5\(^5\).\(^5\(^6\).\(^5\(^7\).\(^5\(^8\).\(^5\(^9\).\(^6\(^0\).\(^6\(^1\).\(^6\(^2\).\(^6\(^3\).\(^6\(^4\).\(^6\(^5\).\(^6\(^6\).\(^6\(^7\).\(^6\(^8\).\(^6\(^9\).\(^7\(^0\).\(^7\(^1\).\(^7\(^2\).\(^7\(^3\).\(^7\(^4\).\(^7\(^5\).\(^7\(^6\).\(^7\(^7\).\(^7\(^8\).\(^7\(^9\).\(^8\(^0\).\(^8\(^1\).\(^8\(^2\).\(^8\(^3\).\(^8\(^4\).\(^8\(^5\).\(^8\(^6\).\(^8\(^7\).\(^8\(^8\).\(^8\(^9\).\(^9\(^0\).\(^9\(^1\).\(^9\(^2\).\(^9\(^3\).\(^9\(^4\).\(^9\(^5\).\(^9\(^6\).\(^9\(^7\).\(^9\(^8\).\(^9\(^9\).\(^0\(^0\).\(^0\(^1\).\(^0\(^2\).\(^0\(^3\).\(^0\(^4\).\(^0\(^5\).\(^0\(^6\).\(^0\(^7\).\(^0\(^8\).\(^0\(^9\).\(^1\(^0\).\(^1\(^1\).\(^1\(^2\).\(^1\(^3\).\(^1\(^4\).\(^1\(^5\).\(^1\(^6\).\(^1\(^7\).\(^1\(^8\).\(^1\(^9\).\(^2\(^0\).\(^2\(^1\).\(^2\(^2\).\(^2\(^3\).\(^2\(^4\).\(^2\(^5\)).
In this Brief Communication, we have developed a microscopic moiré spin Hamiltonian to describe the MMEIs in twisted magnets via a sliding-mapping approach. We demonstrate that the appearance of MMEIs can induce a type of magnetic skyrmion bubble (SKB) with non-conserved helicity in tBL-CrI₃. We name this ‘moiré-type SKBs’. Interestingly, by finely tuning the small $\theta$, the size and population of these moiré-type SKBs can be precisely controlled. Furthermore, we reveal that substrate-induced interfacial Dzyaloshinskii–Moriya (DM) interactions can largely modulate the intrinsic MMEIs and, in turn, govern the $\theta$-dependent MPTs. This can solve the outstanding disagreements between prior theories and experiments in tBL-CrI₃. Our study provides a benchmark for understanding MMEIs and unusual MMEI-induced physics.

A general moiré spin Hamiltonian includes the site-dependent MMEIs as follows:

$$H = \sum_{ij} J_{\text{inter}}^{ij} S_i \cdot S_j + \sum_{ij} J_{\text{intra}}^{ij} S_i \cdot S_j + \sum_{ij} D_{\text{inter}}^{ij} (S_i \cdot S_j)$$

$$+ \sum_{i} D_{\text{intra}}^{i} (S_i \cdot S_j) + K \sum_{i} (S_i^2)^2 + H_{\text{ext}}$$

(1)

where $S_i$ and $S_j$ are spin operators at sites $i$ and $j$; $J_{\text{inter}}^{ij}$ and $J_{\text{intra}}^{ij}$ represent the interlayer and intralayer Heisenberg exchange couplings; $D_{\text{inter}}^{ij}$ and $D_{\text{intra}}^{i}$ represent the interlayer and intralayer DM exchange couplings. $K$ indicates the effective strength of the single-ion anisotropy. $H_{\text{ext}}$ is the external interaction term induced by external fields or substrate effect. The summations for $i$ and $j$ run over all neighboring Cr atoms within the length scale of the Cr-Cl unit cell. As discussed in the Methods and Extended Data Fig. 1, we have developed a sliding-mapping approach to solve these MMEI parameters.

We first use an example of $\theta = 1.41^\circ$ to discuss the magnetic properties of tBL-CrI₃, which can generate a commensurate moiré superlattice with 53,024 atoms and 198,528 nonequivalent MMEI parameters. Starting from equation (1), the Landau–Lifshitz–Gilbert equation is used to solve the classical atomic spin problem in tBL-CrI₃. Figure 1a shows that there are several circular spin textures with two major different sizes distributed in the moiré superlattice. Surprisingly, these two types of circular spin textures are layer dependent with opposite spin swirling structures. The distributions of normalized magnetic moments along the diameter of circular texture reveal that the moments in the inner and outer regions of these textures are upwards and downwards (Supplementary Fig. 1), respectively, which clearly shows that these microstructures are SKBs. The inner and outer diameters of the SKB are ~2.4 and ~9.6 nm, respectively, much smaller than typical SKBs of several hundred nanometers.

We found that these SKBs solely appear around local AB-stacking sites in the moiré lattice, implying that MMEIs may have a strong correlation with the distribution of these SKBs. As shown in Extended Data Fig. 1e, $D_{\text{inter}}$ is nearly constant and is much larger than other magnetic parameters. Therefore, $D_{\text{inter}}$ is a relatively small value and negligible. Contrastingly, as shown in Fig. 1b, the $D_{\text{intra}}$ values surrounding the AB-stacking sites (marked by the dashed-white circle, referred to hereafter as DWC) are much larger than at other sites, and could be sufficiently strong to generate noncollinear spin textures (see enlarged DWC structure in Supplementary Fig. 2). Interestingly, if only the shortest range, nearest (1N) MMEIs are considered (Fig. 1c), instead of SKBs, only collinear ferromagnetic (FM) configurations can be generated (see Supplementary Fig. 3), as the $D_{\text{intra}}^\text{IN}$, $J_{\text{intra}}^\text{IN}$ cannot capture the long-range MMEIs. In other words, the MMEIs at local sites are strongly correlated with the MMEIs at long-range sites.

To further demonstrate the strong correlation between local and long-range sites in MMEIs: (I) we artificially built a BL-CrI₃ with a stacking style similar to the DWC region shown in Fig. 1d; that is, with long-range MMEIs completely removed. Interestingly, no non-collinear spin textures were generated (Supplementary Fig. 4); (2) we plotted $J_{\text{inter}}$, $D_{\text{inter}}$, and $D_{\text{inter}}/J_{\text{inter}}$, which were averaged over the DWC region. As shown in Fig. 1d, only when the >4N MMEIs were considered, could a converged $D_{\text{inter}}/J_{\text{inter}}$ be obtained. Only if the >4N MMEIs were considered, could SKBs similar to Fig. 1a be generated (Supplementary Fig. 3). Therefore, both short-range and long-range MMEIs are critical for describing the local complex spin textures in twisted magnets.

In general, three physical quantities (topological number ($N_\theta$), vorticity ($\omega$) and helicity ($\gamma$); Supplementary Section I) can be used to distinguish magnetic skyrmions and SKBs. For tBL-CrI₃, $N_\theta$ and $\omega$ for both top and bottom SKBs are −1 and 1, respectively. Unexpectedly, $\gamma$ becomes non-conserved, that is, it changes with the azimuthal angle, $\phi$ (Fig. 1e), which has never been observed or predicted in existing skyrmions. Therefore, we term it moiré-type SKB, reflecting a unique spin texture solely generated by MMEIs. The calculated $\gamma$ for top and bottom SKBs are in ranges of [15°, 37°] and [−148°, −114°], respectively, that is, they are near opposite (different by $\pi$) each other, due to the opposite $D$ for distinct layers at the same stacking sites. Interestingly, $\gamma$ can be fitted by trigonometric function as:

$$\gamma = \sum_n (A_n \sin n\phi + B_n \cos n\phi) + C_0,$$

(2)

where $A_n$, $B_n$, $A_2$, $B_2$, $C_0$ and $\omega$ for top (bottom) SKBs are 3.34, −8.11, −1.88, −1.70, 27.18, and 0.018 (0.77, −16.42, −0.10, −1.62, −127.50 and 0.013), respectively. While $C_0$ approximates the average $\gamma$, $A_n$, $B_n$ and $\omega$ describe the deviation from averaged $\gamma$ at different $\phi$. This non-conserved $\gamma$ may induce unconventional physical phenomena.

The origin of non-conserved $\gamma$ is interesting. According to the Moriya rule, $D$ is parallel (perpendicular) to the line connecting two magnetic atoms for a $D_C (D_A)$ point group. And minimizing corresponding DM energy in the Lifshitz invariants results in Bloch-type (Néel-type) skyrmions with helicity of ±90° (0° or 180°) in a $D_C (D_A)$ point group (Supplementary Fig. 5). As shown in Fig. 1f, for $C_\text{ct}$ point group crystals that can be regarded as a subgroup of $D_C$ and $C_{\text{nn}}$, there is an angle between the DM vector and $\gamma$. Accordingly, the Lifshitz invariants consist of terms with simultaneous presence of DM interaction with both $x$ and $y$ components and the corresponding helicity is $\gamma = \arctan (D_x/D_y)$. For example, the corresponding spin texture with $D_x = −1$ and $D_y = 1$ is plotted at the bottom of Fig. 1f. However, in the tBL-CrI₃ system, although the global symmetry belongs to the $C_{\text{ct}}$ point group, the MMEIs can produce the unique non-conserved $\gamma$ character in the twisted magnets.

To further distinguish the role of MMEIs in contributing to the non-conserved $\gamma$, both $D_{\text{inter}}$ and $D_{\text{intra}}$ at the DWC region for the top and bottom layers of tBL-CrI₃, are plotted in Fig. 1g. The local $D_{\text{inter}}$ is a near uniform value and gradually winds around the DWC region, resulting in the $\gamma$ near a constant value but deviation from 0°, 180° or ±90°. Therefore, the $D_{\text{intra}}$ of MMEIs determines the $C_\theta$ in equation (2), while the local $D_{\text{intra}}$ is randomly distributed around the DWC region, resulting in the $\gamma$ deviation from a constant value and determining the $A_n$, $B_n$, and $\omega$ in equation (2). $D_{\text{intra}}$ plays a key role in forming non-conserved $\gamma$.

As demonstrated in Fig. 1h, it is interesting to further understand the basic rules of the interactions between SKBs in the same layer or different layers. SKBs located in the same layer have the same sign of $\gamma$. Accordingly, the differential of potential $U$ as a function of the distance $R$ between two SKBs in the same layer is always negative (Fig. 1h), giving rise to a repulsion between two neighboring SKBs (for example, SKB1 and SKB2 in Fig. 1h). SKBs located in different layers have opposite sign of $\gamma$. As shown in Fig. 1h, if the two SKBs are far from each other, there is an attraction between them (for example, SKB1 and SKB3 in Fig. 1h); if two SKBs are close to each other, there will be a much stronger repulsion between them (for example, SKB1 and SKB4 in Fig. 1h). Therefore, SKBs in top and bottom layers cannot appear at the same stacking site.
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Fig. 1 | MMEI-induced moiré-type SkBs at θ ~ 1.41°. a, Spin texture in tBL-CrI₃ at θ ~ 1.41°. Insets show the SkBs in the top and bottom layers. The rectangular unit cell of the moiré superlattice is shown by the dashed-red line. b, c, Color mapping for MMEIs ($D_{\text{intra}}/I_{\text{intra}}$) including tenth-nearest (10N; b) and nearest (1N; c) magnetic interactions. d, Average $f_m$,$D_{\text{intra}}$ and $D_{\text{intra}}/I_{\text{intra}}$ around the dashed-white circle (DWC) region (in b) as a function of a range of magnetic interactions. e, Helicity (γ) as a function of azimuth angle (φ), indicating the ϕ dependence.

Fig. 2a, when $\theta$ < 1.20°, the moiré pattern becomes clear with maximum values at the DWC region around AB-moiré (in Fig. 2b). Whereas, as $\theta$ decreases, the MMEI patterns appear and become clear with maximum values at the DWC region around AB-moiré. Therefore, $N/N_{\text{moire}}$ increases as a function of $\theta$ decreases from 2.00° to 1.30°. Meanwhile, as $\theta$ decreases, the diameters of SkBs monotonously enlarge (Fig. 2c), but the domain wall width remains at ~3 nm as $\theta$ decreases (Supplementary Fig. 9). Overall, the non-conserved γ is observed in all the SkBs at different $\theta$ values, showing similar features as that at 1.41° (Supplementary Fig. 6e). Therefore, $\theta$-controlled MMEIs play a key role in determining the population and size of SkB.

It is interesting to further investigate the role of external substrate on modulating MMEIs, as the substrate further reduces the symmetry of tBL-CrI₃. As indicated in Fig. 2d, taking experimentally used layered BN substrate as example, the substrate-induced interfacial DM ($D_{\text{sub}}$) further modulates the MMEIs, changing the $\theta$-dependent MPTs. Given the complexity of the real CrI₃/BN interface, we approximate this interfacial DM as a typical value in the range of ~0.71–0.87 meV per Cr, based

(Fig. 1a and Supplementary Fig. 6). The competition between SkB–SkB repulsive and attractive interactions between different layers in the triangular moiré lattice could induce an SkB frustrated lattice that has not been observed before (Supplementary Fig. 7).

Similarly, we have systematically investigated spin textures in tBL-CrI₃ with other commensurate $\theta$ values ranging from 21.78° to 0.99°. In these systems, the number of nonequivalent MMEI parameters varies in a range of ~832–403,548. Some representative results are shown in Fig. 2a. When $\theta$ > 2.00°, only ordinary moiré patterns with FM spin textures are observed (Supplementary Fig. 8). When $\theta$ = 2.00°, the moiré-type SkBs start to appear, whose numbers increases as $\theta$ decreases. In particular, when $\theta$ < 1.30°, each DWC region in the moiré unit cell can generate one noncollinear spin texture, which can be SkB or circular domains or antiskyrmions (Supplementary Figs. 6a–d). The ratio of noncollinear spin texture in one moiré unit cell ($N/N_{\text{moire}}$) is summarized in Fig. 2b. At a large $\theta$, there are few magnetic atoms in the moiré unit cell, as a result, the $D_{\text{intra}}/I_{\text{intra}}$ cannot form clear MMEI patterns to generate noncollinear spin textures (for example, right inset for $\theta$ ~13.17° in Fig. 2b). Whereas, as $\theta$ decreases, the MMEI patterns appear and become clear with maximum values at the DWC region around AB-stacking positions. As shown in Fig. 2b, from left inset with $\theta$ ~1.20° to middle inset with $\theta$ ~2.00°, the smaller the $\theta$, the sharper the MMEI pattern. Therefore, $N/N_{\text{moire}}$ increases as a function of $\theta$ decreases from 2.00° to 1.30°. Meanwhile, as $\theta$ decreases, the diameters of SkBs monotonously enlarge (Fig. 2c), but the domain wall width remains at ~3 nm as $\theta$ decreases (Supplementary Fig. 9). Overall, the non-conserved γ is observed in all the SkBs at different $\theta$ values, showing similar features as that at 1.41° (Supplementary Fig. 6e). Therefore, $\theta$-controlled MMEIs play a key role in determining the population and size of SkB.

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on several typical interfacial configurations (Supplementary Fig. 10 and Supplementary Table 1), which is at least five times larger than the maximum $D_{\text{ intra}}$ in tBL-CrI$_3$. Therefore, the substrate may have a strong influence on the spin textures of tBL-CrI$_3$. In the following, the external interaction term

$$H_{\text{ext}} = D_{\text{sub}} \sum_{i,j} (S_i \times S_j)$$  \hspace{1cm} (3)$$

is used in equation (1) to simulate the substrate effect.

Figure 2e shows the magnetic phase diagram as a function of $D_{\text{sub}}$ and $\theta$ (Supplementary Fig. 11 for detailed spin textures). (1) For large $\theta$, when $D_{\text{sub}}$ is not sufficiently strong, the MMEIs cannot exhibit significant changes. For example, inset (iv) shows a typical FM spin texture with $D_{\text{sub}} = 0$ and $\theta = 3.15^\circ$. When the influence of $D_{\text{sub}}$ is sufficiently strong, the spins will tilt and the tBL-CrI$_3$ exhibits the magnetic domains for large $\theta$. For example, inset (ii) shows a typical spin texture with $D_{\text{sub}} = 1.00$ meV and $\theta = 3.15^\circ$. (2) For relatively small $\theta$, the MMEIs become more important (Fig. 2b), as a result, the SkBs appear. For example, inset (iii) shows an SkB with $D_{\text{sub}} = 0$ and $\theta = 1.41^\circ$. Importantly, with the assistance of strong $D_{\text{sub}}$, the $D_{\text{sub}}$-modulated MMEIs together with the coulomb repulsion between different SkBs leads to the appearance of trivial bubbles (not SkBs) not only around the AB stacking (that is, DWC) regions but also around the AA and BA stacking areas, forming the unexpected hexagonal patterns. For example, inset (i) shows the trivial bubbles with $D_{\text{sub}} = 0.80$ meV and $\theta = 1.20^\circ$. This is because, via the $D_{\text{sub}}$ term, besides around AB stacking, the $D/J$ around AA and BA stacking sites can also significantly enlarge, as shown in Fig. 2f, which is beneficial for the appearance of the noncollinear spin textures, eventually forming hexagonal patterns. Furthermore, the sizes of these trivial bubbles are >10 nm and the averaged magnetic moment is about 0.7 times the saturation magnetism ($M_s$) of CrI$_3$. Overall, as indicated in Fig. 2e, by tuning $D_{\text{sub}}$ via different substrates, in principle, different MPTs can be achieved in twisted magnets.

The conditions for the experimentally observed FM region and FM–AFM-coexisting region with hexagonal spin textures in tBL-CrI$_3$, are labeled as up and down triangles in Fig. 2e, respectively. Interestingly, these two spin textures fall into (iv) and (i) regions, agreeing with our calculations. In particular, the transition region (marked as a square) between $\theta = 2–3^\circ$ is very similar to the experimentally observed critical point with the coexistence of FM and FM–AFM phases\(^{15}\), indicating that the hexagonal periodic noncollinear spin textures observed in...
experiments at small $\theta$ could be essentially the trivial magnetic bubbles. Interestingly, in this transition region, the unconventional moiré-type SKBs can also exist, which is likely to be detected in the current experimental samples, opening an opportunity to explore moiré-type SKB-related physics.

Although our proposed moiré spin Hamiltonian via the sliding-mapping method can describe MMEIs and solve the disagreement between existing theories and experiments, due to the difference between sliding and rotation in reality, this method is more suitable for the systems with small twisted angles (see details in Methods). In addition, we note that the anisotropic Kitaev and other small high-order magnetic interactions are not included in our present study, which may deserve further studies on their roles in twisted magnets.

## Methods

### Sliding-mapping method for MMEIs

The long-periodic moiré pattern in tBL-CrI$_3$ is formed by twisting one monolayer with respect to the other one with a small $\theta$, as shown in Extended Data Fig. 1a. Importantly, the local crystal structures in the moiré pattern are nearly equivalent to a series of BL-CrI$_3$ by smoothly sliding the top layer by a vector $\mathbf{r} = \mathbf{m}_a + \mathbf{n}_a$, with respect to bottom layer from the AA-stacking structure, as shown in Extended Data Fig. 1b, where $\mathbf{a}_i$ is the in-plane unit vectors of the monolayer CrI$_3$. For example, the surrounded insets of Extended Data Fig. 1a show four typical local crystal structures, that is, AB, BA, AB$'$ and BA$'$, whose interlayer sliding vectors are $(\mathbf{m}, \mathbf{n}) = (0, 0), (2/3, 2/3), (1/3, 1/3)$ and $(0, 1/3)$, respectively. The most general moiré spin Hamiltonian should include all the site-dependent MMEIs, as shown in equation (1).

While directly solving the parameters in equation (1) is very unlikely, we have instead developed a sliding-mapping approach to solve these MMEI parameters. Extended Data Fig. 1c shows a typical example to calculate the $J_{\text{inter}}$ in tBL-CrI$_3$. The middle panel shows the enlarged local atomic structure of tBL-CrI$_3$ marked as the blue frame region in Extended Data Fig. 1a. Here, four typical inter-atomic $J_{\text{inter}}$ with different distance $r(r_1, r_2, r_3, \ldots)$ are labeled. To obtain the $J_{\text{inter}}(r)$ between two Cr atoms in tBL-CrI$_3$, we first determine the distance $r$ between the two Cr atoms; second, in BL-CrI$_3$, sliding the top layer CrI$_3$ with respect to the bottom layer with the vector $\mathbf{r}$, we can see the local atomic position in tBL-CrI$_3$ around with respect to the bottom layer with the vector $\mathbf{r}$, we can see the local atomic position in tBL-CrI$_3$. The middle panel shows the local crystal structures, that is, AB, AA, AB and BA, whose interlayer sliding vectors are $(\mathbf{m}, \mathbf{n}) = (0, 0), (2/3, 2/3), (1/3, 1/3)$ and $(0, 1/3)$, respectively. The most general moiré spin Hamiltonian should include the site-dependent MMEIs, as shown in equation (1).

In short, as the local structures in tBL-CrI$_3$ are equal to that of BL-CrI$_3$ generated via smooth sliding, the magnetic parameters between two Cr atoms at each local site in the tBL-CrI$_3$ ($D$ and $J$) could be effectively derived through mapping the magnetic parameters of BL-CrI$_3$ ($D_{\text{inter}}$ and $J_{\text{inter}}$) by smoothly changing the sliding vector $\mathbf{r}$ (Supplementary Information Section 2). In principle, as long as the sliding process is sufficiently smooth, one could always get an approximate one-to-one correspondence of the magnetic parameters between BL-CrI$_3$ and tBL-CrI$_3$. In particular, the smaller the $\theta$, the more accurate the mapping parameters one could obtain. Therefore, this approach is very suitable for the twisted magnets that usually have very small $\theta$. Because it is impossible to consider all the MMEIs under $(\mathbf{m}, \mathbf{n}) > 1$ and also because the strength of MMEIs will rapidly decrease for larger $\mathbf{m}$ and $\mathbf{n}$, only the MMEIs within the $(\mathbf{m}, \mathbf{n}) \leq 1$ region are considered to ensure the interlayer (nearest to tenth-nearest neighboring) $J_{\text{inter}}$, $J_{\text{inter}}$ and $J_{\text{inter}}$ ($\mathbf{m}, \mathbf{n}$) and $J_{\text{inter}}$, $J_{\text{inter}}$ and $J_{\text{inter}}$ ($\mathbf{m}, \mathbf{n}$) couplings in a hexagonal lattice are fully included in the moiré superlattice (see Supplementary Fig. 12).

### Magnetic interactions in BL-CrI$_3$ with different stackings

The magnetic interactions in BL-CrI$_3$ with different sliding vectors $\mathbf{r}$ are plotted in Extended Data Fig. 1d–h. The calculated interlayer exchange $J_{\text{inter}}$ is mostly FM ($D > 0$) but with three AFM ($D < 0$) patches within the unit cell (Extended Data Fig. 1d). However, unlike with previous models, three important features of $J_{\text{inter}}$ can be observed. (1) $J_{\text{inter}}$ differs when the top layer slides to $(\mathbf{m}, \mathbf{n}) = (1, 0)$ and $(1, 1)$. Because the Cr$_x$ symmetric point group of AA-stacking BL-Crl$_3$ lacks $\sigma_y$ symmetry operation, the exchange path between Cr$_1$ in the bottom layer and Cr$_2$ and Cr$_3$ in the top layer, that is, Cr$_1$–Cr$_2$, and Cr$_1$–Cr$_3$, pairs (marked in Extended Data Fig. 1a), differs from each other. (2) The $J_{\text{inter}}$ shows $c_z$ but not $c_x$ rotation symmetry due to the same reason. (3) Except in the AFM patch regions, $J_{\text{inter}}$ gets smaller as a function of sliding vector $\mathbf{r}$, which is due to the decreased exchange integral as the distance between two interlayer Cr atoms increases. For intralayer exchange coupling, the relative positions of the three nearest and six next-nearest neighboring intralayer Cr–Cr pairs are not changed, but their exchange paths are influenced by the sliding vector $\mathbf{r}$. Therefore, $\sigma_{\text{c}_1}$ (Extended Data Fig. 1e) and $\sigma_{\text{c}_2}$ (Extended Data Fig. 1f) are not homogeneous anymore, although without the dramatic changes with the sliding vector $\mathbf{r}$. Similarly, $\sigma_{\text{c}_3}$ rotation symmetry is also observed in the $J_{\text{inter}}$ and the $\sigma_{\text{c}_4}$ slightly changes compared with that of $J_{\text{inter}}$.

The symmetry of AA-stacking BL-CrI$_3$ breaks when the top layer Cr$_1$ slides as a function of $\mathbf{r}$, leading to the emergence of DM interaction. Similar to $J_{\text{inter}}$, the interlayer DM $D_{\text{inter}}$ can also be influenced by the intralayer stackings, as shown in Extended Data Fig. 1g. The $x$ and $y$ components ($D_{\text{inter}}$ and $D_{\text{inter}}$) show the symmetric and antisymmetric features with respect to the $x$ axis. This is because for an arbitrary site $\mathbf{r}$ with the corresponding sliding vector $\mathbf{r}$ (Extended Data Fig. 1h), we could first rotate site 1 counterclockwise by 120° to site 3 and then perform the mirror operation with respect to the $y$ plane to get the site 2, that is, sites 1 and 2 are symmetric along the $x$ axis. Therefore, $D_{\text{inter}}(2) = 0 \times R_{120} \times D_{\text{inter}}(1)$, where $\sigma = (−1/2$, $\sqrt{3}/2$, $1/2)$, $R_{120} = (−1/2$, $\sqrt{3}/2$, $−1/2)$, leading to $D_{\text{inter}}(2) = D_{\text{inter}}(1)$ and $D_{\text{inter}}(2) = D_{\text{inter}}(1)$. Different from the in-plane components, the $D_{\text{inter}}$ shows $c_z$ symmetry. The overall next-nearest intralayer DM $D_{\text{inter}}$ is much weaker than that of nearest intralayer DM $D_{\text{inter}}$ (Supplementary Fig. 13). Therefore, Extended Data Fig. 1i only presents the nearest intralayer DM vector $D_{\text{inter}}$ and $D_{\text{inter}}$. The $J_{\text{inter}}$ and $D_{\text{inter}}$ show similar symmetry compared with $J_{\text{inter}}$ and $D_{\text{inter}}$ but the $c_z$ symmetry for $D_{\text{inter}}$ is not maintained anymore. Surprisingly, although the interlayer distance between two neighboring Cr atoms is significantly larger than that in the intralayer one, the magnitude of $D_{\text{inter}}$ is comparable to that of $D_{\text{inter}}$. This unexpected finding is possibly because during the sliding of top layer, the local symmetry of intralayer is less reduced compared with that of interlayer symmetry. Therefore, solely considering $D_{\text{inter}}$ but neglecting $D_{\text{inter}}$ in twisted moiré magnets may be incorrect to describe the magnetic properties of twisted moiré magnets.

Overall, in BL-CrI$_3$, $J_{\text{inter}}$ and $D_{\text{inter}}$ are almost three and more than ten times larger than $J_{\text{inter}}$ and $D_{\text{inter}}$, respectively. Furthermore, the calculated perpendicular magnetic anisotropy of Cr atoms is 0.866 meV per Cr. Differing from conventional magnets with homogeneous magnetic interactions, the MMEIs in twisted magnets may exhibit a noticeable site-dependent feature, which is further tunable by $\theta$ and $H_{\text{ext}}$ (equation (1)). Consequently, the competition between $D$ and $J$ varies at different site of the moiré system, that is, it is possible to generate the noncollinear spin textures at specific local positions in the moiré pattern of tBL-CrI$_3$.

## DFT calculations

The DFT calculations are performed using the Vienna Ab Initio Simulations Package (VASP.6.1.2). The core electrons were treated using the projector augmented wave (PAW) method and the correlation potential was treated using the generalized gradient approximation (GGA) with the standard Perdew–Burke–Ernzerhof (PBE) pseudopotential. The optB86b van der Waals correction was employed in all calculations. Dudarev’s method with an effective Hubbard $U = 3.0$ eV was used to correct the correlation effects caused by the partially occupied Cr-3d orbitals. A 300 eV energy cutoff and a $9 \times 9 \times 1$ Γ-centered $k$-mesh were adopted to perform calculations. To avoid the artificial interaction
caused by periodic boundary conditions, a vacuum of 15 Å was added. The in-plane lattice constant of BL-CrI$_3$ was fixed to 6.93 Å for different stacking models. All the atoms were fully relaxed along the $z$-direction in bilayer CrI$_3$ system until the force and total energy was less than 0.01 eV Å$^{-1}$ and 10$^{-5}$ eV. In our simulation, we construct the CrI$_3$/BN heterojunction with 1 × 1 CrI$_3$ lattice and 3 × 3 BN.

To remove the artificial strain effect in the twisted bilayer systems, only commensurate values were considered. The atomic positions in tBL-CrI$_3$ moiré crystal were mapping from the different stacking structures. The magnetic interactions, including exchange interaction $J$ and $D$, were calculated based on the Green’s function method $\text{10}$. The single-ion anisotropy was calculated using the force theorem. The tBL-CrI$_3$ in our calculation with largest twisted angle 21.78 degrees and smallest twisted angle 0.99 degrees contain 28 (832) and 13,468 (403,548) magnetic Cr atoms (MME parameters), and the corresponding lattice constants were 18.34 Å and 402.12 Å, respectively.

Atomic spin simulations

The spin dynamics simulations were performed using the VAMPIRE package. The time evolution of the magnetization was described by the Landau–Lifshitz–Gilbert equation and was integrated numerically using the Heun numerical scheme. Here, to have a more convenient and higher efficient calculation on the tBL-CrI$_3$ spin textures, the least integral multiple of the rectangular moiré lattices with the size larger than 100 nm x 100 nm was adopted for each system, which contains over 96,000 magnetic atoms. The periodic boundary conditions were used to perform calculations. The initial spin textures were selected as the randomly distributed spin textures. All simulations were performed using the zero-field cool mode which the calculation temperature starts at 30 K and decreases in steps of 1 K to near 0 K. Therefore, the spin textures observed in the tBL-CrI$_3$ are very likely to be the ground-state configurations. For each temperature step, $3 \times 10^6$ calculation steps were performed at a fixed time step of 0.1 fs.

Reporting summary

Further information on research design is available in the Nature Portfolio Reporting Summary linked to this article.

Data availability

The raw data for the first-principles calculations and atomic spin simulations have been deposited in the Zenodo $\text{32}$. Source Data for Figs. 1, 2 and Extended Data Fig. 1 are available with this Paper. Those data are generated by the code developed for this study.

Code availability

The code used in the current study is available at Zenodo $\text{33}$.

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Author contributions
B.H. supervised and led the project. B.Y. and B.H. directed the project. B.Y., Y.L. and B.H. prepared the manuscript. All authors discussed the results and contributed to the manuscript.

Competing interests
The authors declare no competing interests.

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Extended Data Fig. 1 | Generating MMEIs via Sliding-mapping Approach.

a. Moiré superlattice of the tBL-CrI₃. Surrounded insets show the regions with local AA, AB, AB' and BA stackings, where Cr in the top and bottom layers are colored as the gold and blue, respectively. Dashed-yellow line indicates the unit cell of moiré superlattice. Blue frame represents the local site in Extended Data Fig. 1c.
b. Schematic diagram of the relative position of the interlayer Cr atoms with the sliding vector \( \mathbf{r} \).
c. Examples of one-to-one correspondence between \( J_{\text{inter}}(\mathbf{r}) \) in tBL-CrI₃ to \( J_{\text{inter}}(\mathbf{r}) \) in BL-CrI₃ via sliding. Color mapping of d, interlayer exchange interaction \( D_{\text{inter}}^{x} \), e, intralayer nearest-neighboring exchange interaction \( D_{\text{intra}}^{1N} \), f, intralayer next-nearest-neighboring exchange interaction \( D_{\text{intra}}^{2N} \), g, interlayer DM vector \( D_{\text{inter}}^{\text{IN.x}} \), and h, intralayer DM vector \( D_{\text{intra}}^{\text{IN.y}} \) between two Cr atoms as a function of sliding vector \( \mathbf{r} \). Here, all the magnetic parameters are in the unit of meV.
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