Emergence of Meron Kekulé lattices in twisted Néel antiferromagnets

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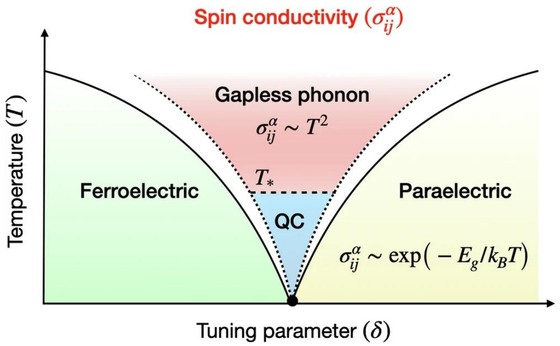
APCTP August 27, 2025

◉ Quantum Matter Theory @ APCTP since 2025.01

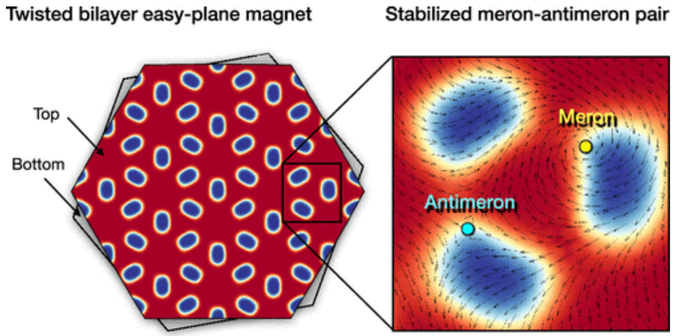
Prof. Kyoung-Min Kim

Dr. Tilen Cadez

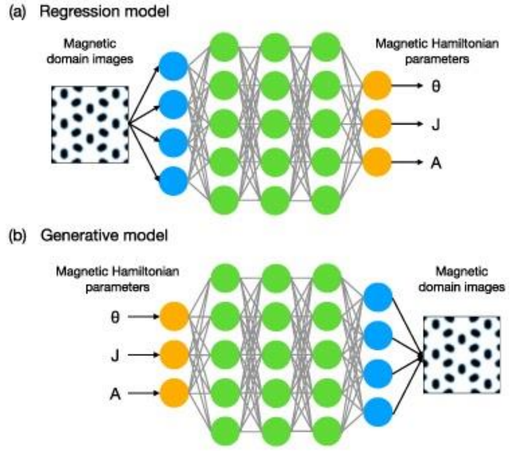
- Correlated electronic systems (Quantum field theory)



- Twisted magnetic layers (Atomistic spin simulation)



- Deep learning (Magnetic domain images)



Outline

I. Twist Engineering of 2D Magnetism

II. Meron Kekulé Lattices in Twisted Antiferromagnets

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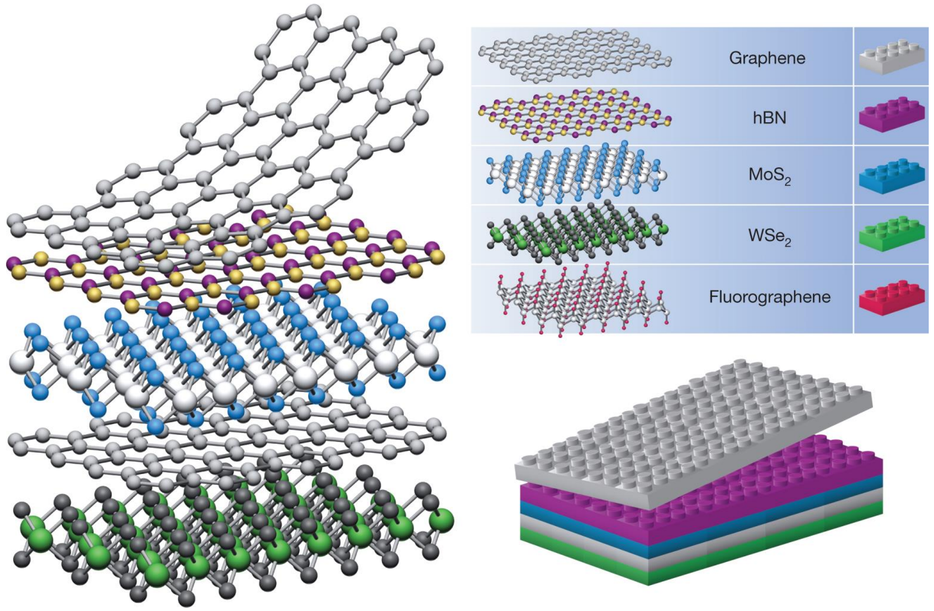
I. Twist Engineering of 2D Magnetism

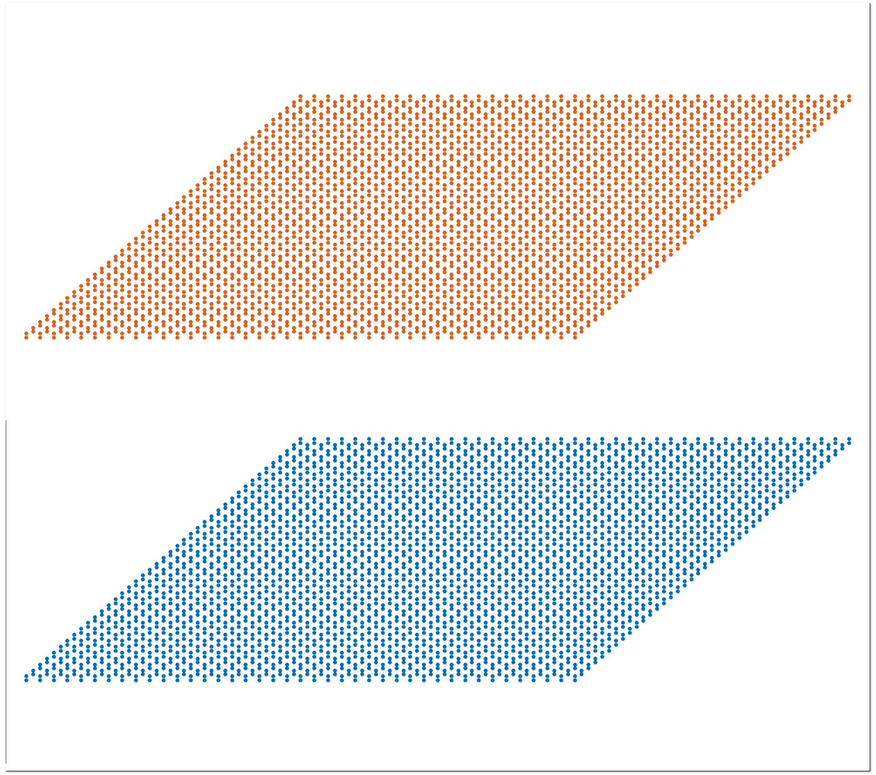
II. Meron Kekulé Lattices in Twisted Antiferromagnets

- **Van der Waals heterostructures**

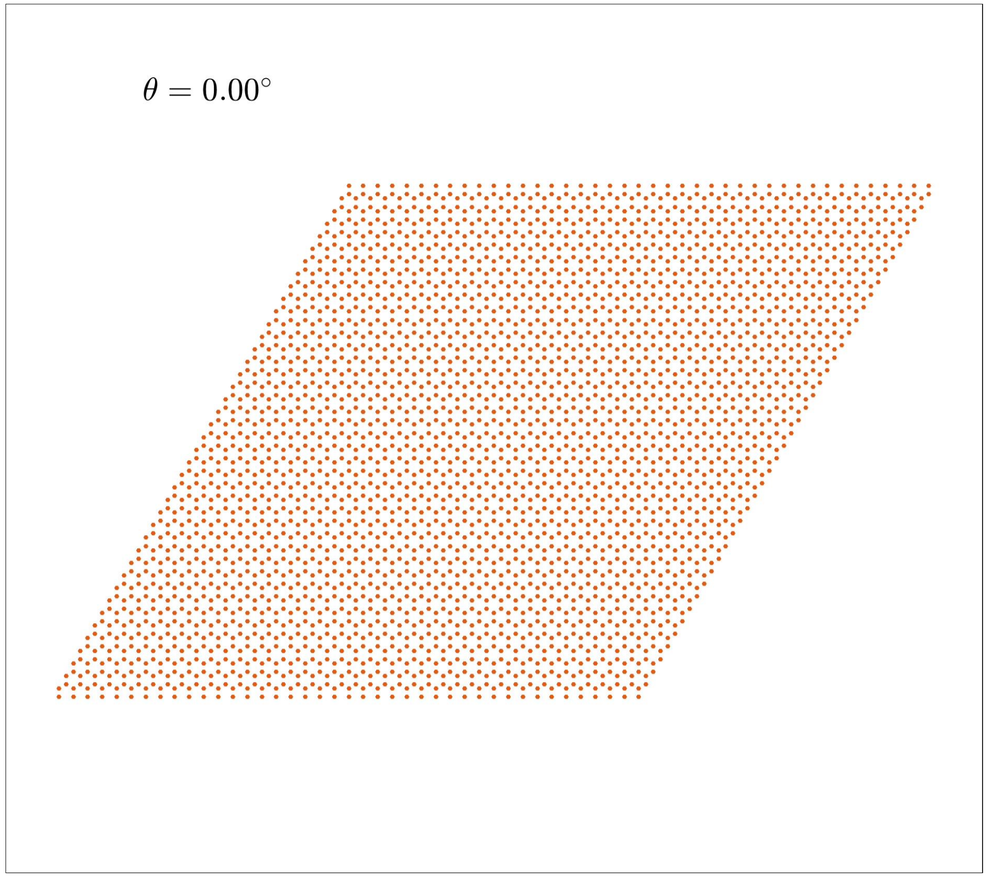


AK Geim & IV Grigorieva Nature 499, 419-425 (2013)

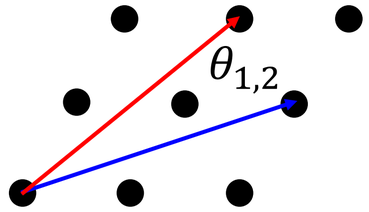
- **Moiré heterostructures**



Commensurate moiré superlattices



- **Commensurate condition**



$\mathbf{R_1} = (1,2)$

$\mathbf{R_2} = (2,1)$

$$\theta_{1,2} = \cos^{-1}\left(\frac{\mathbf{R}_1 \cdot \mathbf{R}_2}{|\mathbf{R}_1||\mathbf{R}_2|}\right) \simeq 21.82°$$

- **Twist angle**

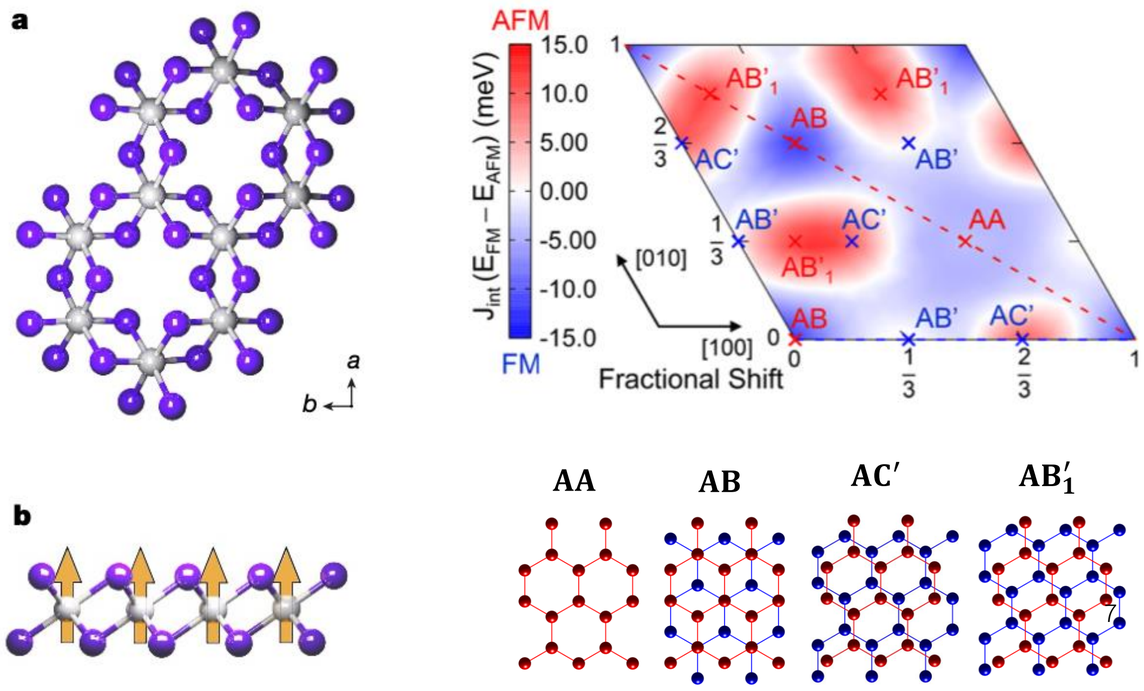
$$\theta_{m,n} = \arccos\left(\frac{m^2 + n^2 + 4mn}{2m^2 + 2n^2 + 2mn}\right)$$

- **Moiré periodicity**

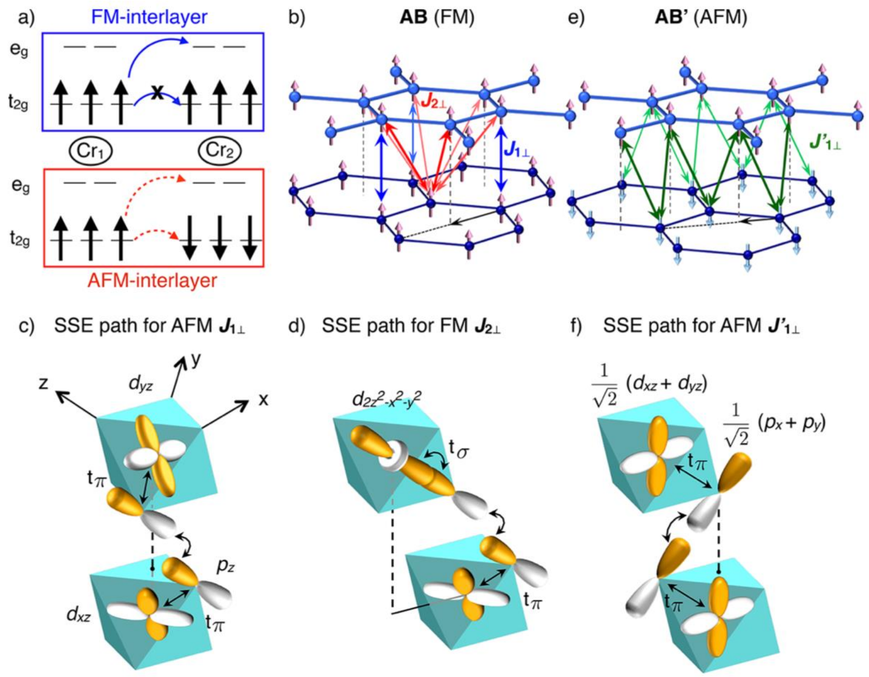
$$L_{m,n} = \frac{a}{2\sin(\theta_{m,n}/2)} \xrightarrow{\theta_{m,n} \ll 1} \frac{a}{\theta_{m,n}}$$

Stacking-dependent interlayer magnetism in CrI3

- **Stacking order → Interlayer Exchange**



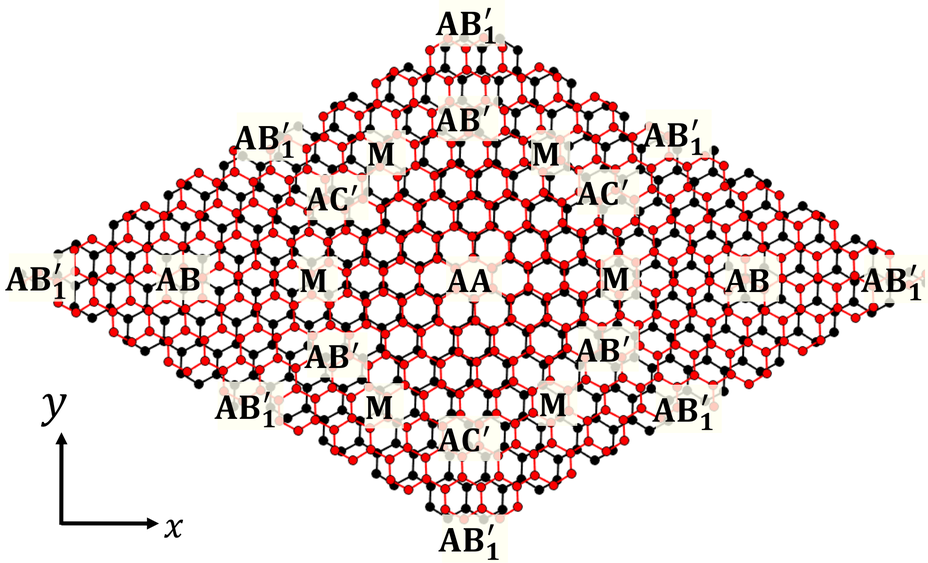
- **Orbital hybridizations → Interlayer Exchange**

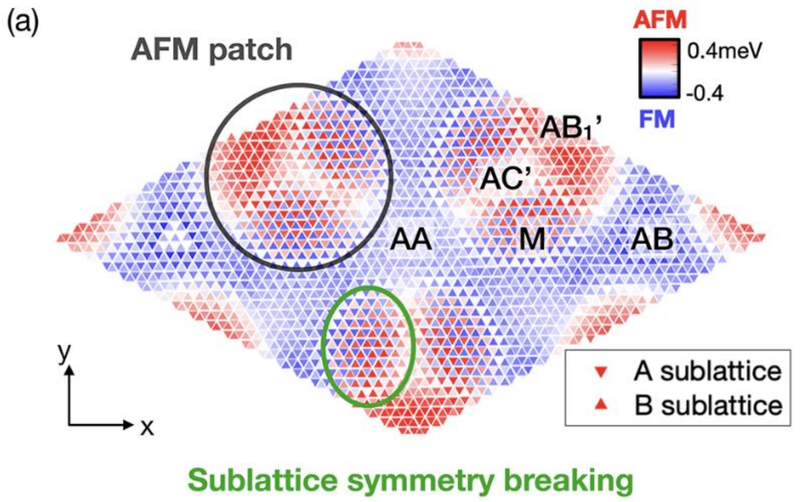


N. Sivadas et al., Nano Letters, 18, 7658 (2018)

Spatial modulation of interlayer exchange

- **Coexistence of various stacking orders**



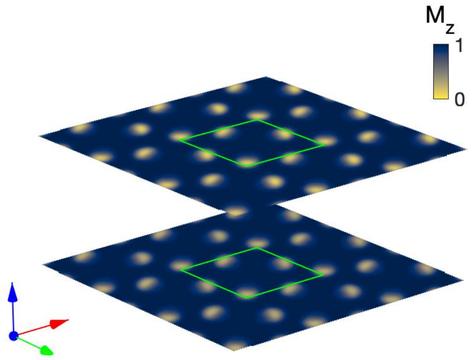


- **Stacking order → Orbital-hybridizations → Interlayer spin interactions**

  - Intralayer spin interactions: stacking-order independent approximately

Moiré magnetism

Non-collinear domain



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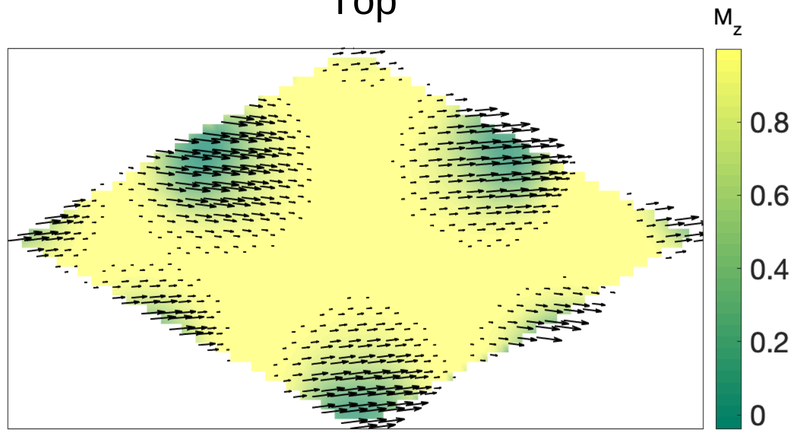

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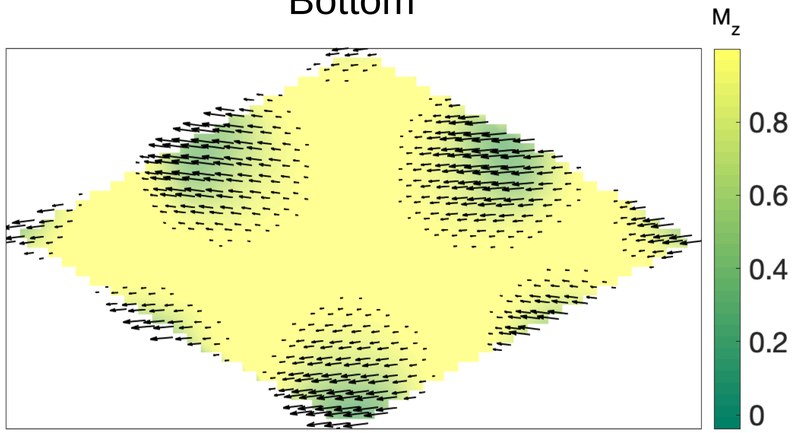
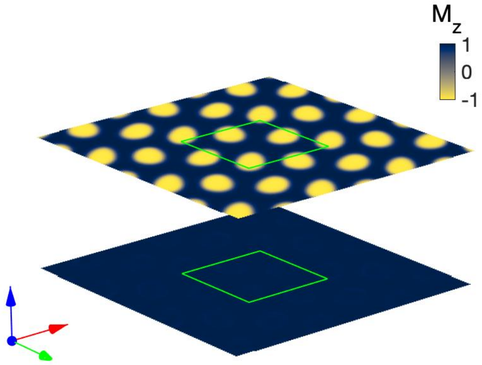


Magnetic domain



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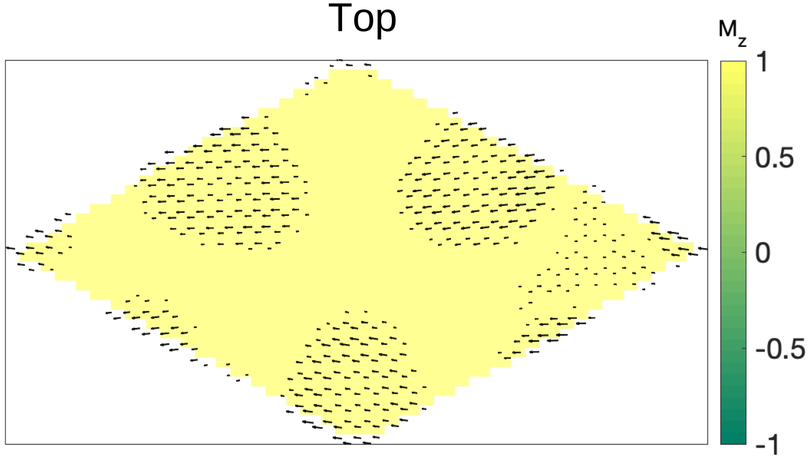

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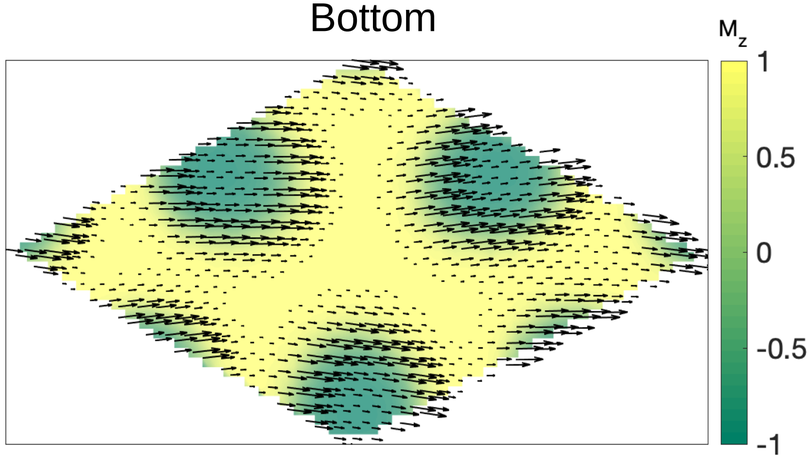
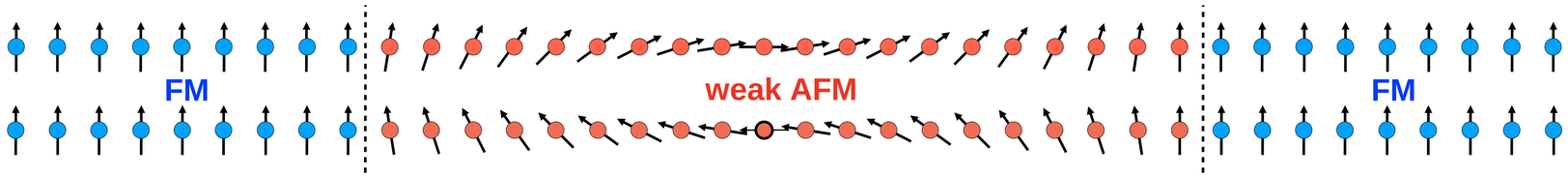


Energetic competition

- **NCD phase**



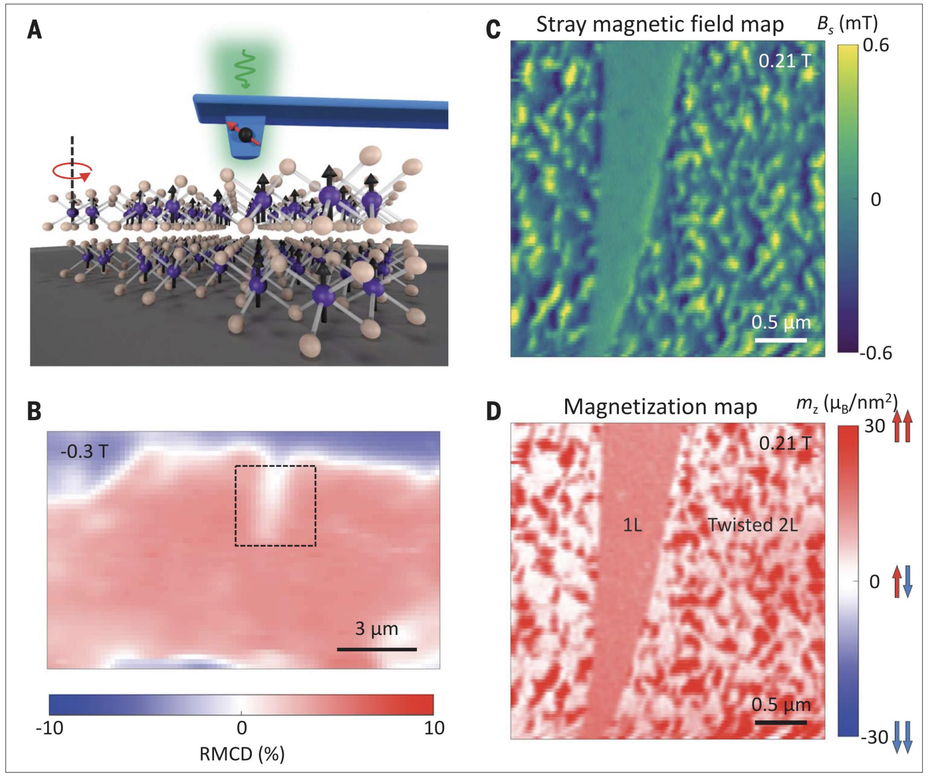
- **MD phase**

- **Gradient energy ($K \sim J > 0$) vs. potential energy ($V \sim -NJ_{\perp} < 0$)**

  - Twist angle controls K-V competition ($N \sim \theta^{-2}$)
  - NCD for $K \sim V$, MD for $K \ll V$

Observation of moiré magnetism

- **AFM measurement in twisted bilayer CrI_3**



T. Song et al., Science, 374, 1140 (2021)

- **Twisted 2D magnets: formation of magnetic domains**

- **What kind of new magnetism in twisted 2D magnets?**

- **How can we study such moiré magnets?**

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What are merons and anti-merons?

- **Merons:** topological spin textures with a half-skyrmion number $Q = -1/2$

- **Skyrmion number:** $Q = \frac{1}{4\pi}\int dx \int dy \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_y \mathbf{n})$

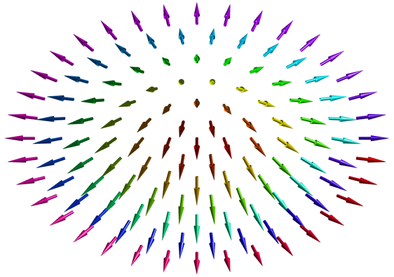
$$\mathbf{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

$$\theta = \theta(r), \phi = \phi(\varphi)$$

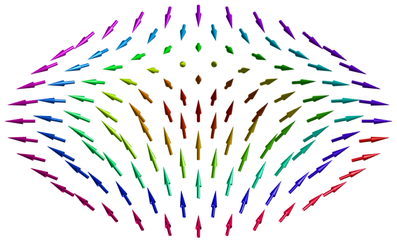
$$Q = p \cdot w$$

- **Polarity:** $p = \frac{1}{2}[\cos\theta(r = \infty) - \cos\theta(r = 0)]$
- **Winding number:** $w = \frac{1}{2\pi}[\phi(\varphi = 0^+) - \phi(\varphi = 0^-)]$

- **Merons:** $Q = -\frac{1}{2}$

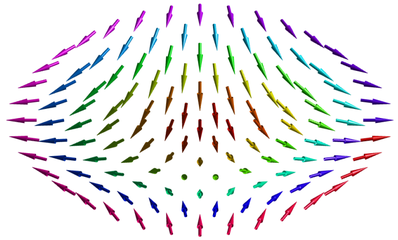


$p = -\frac{1}{2}, w = 1$

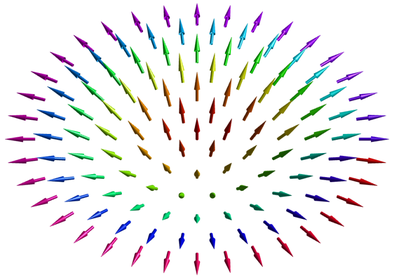


$p = \frac{1}{2}, w = -1$

- **Antimerons:** $Q = +\frac{1}{2}$



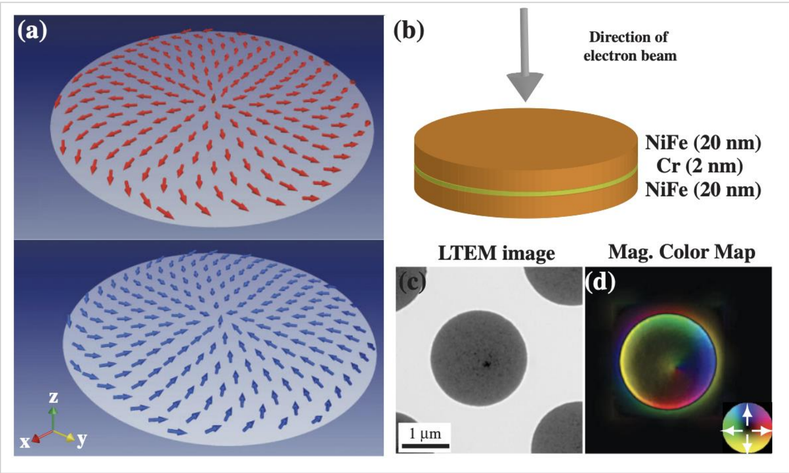
$p = -\frac{1}{2}, w = -1$



$p = \frac{1}{2}, w = 1$

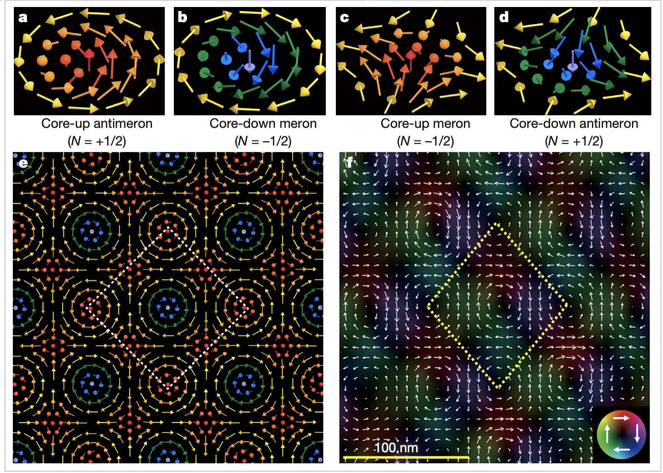
Observation of merons and antimerons in various forms

Isolated forms in magnetic disks (Exp., Py-Cr-Py)



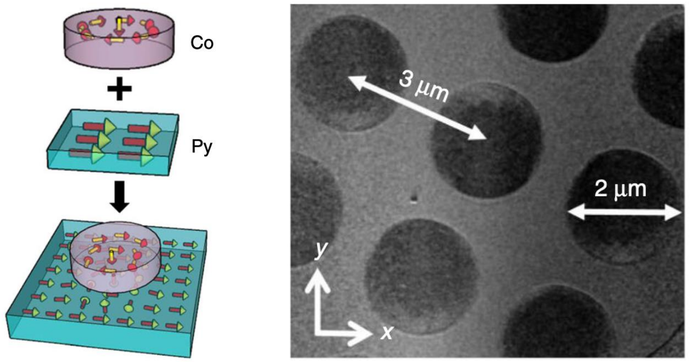
C. Phatak et al., Phys. Rev. Lett. 108, 089901 (2012)

Square lattice in a chiral magnet (Exp., $Co_8Zn_9Mn_3$)



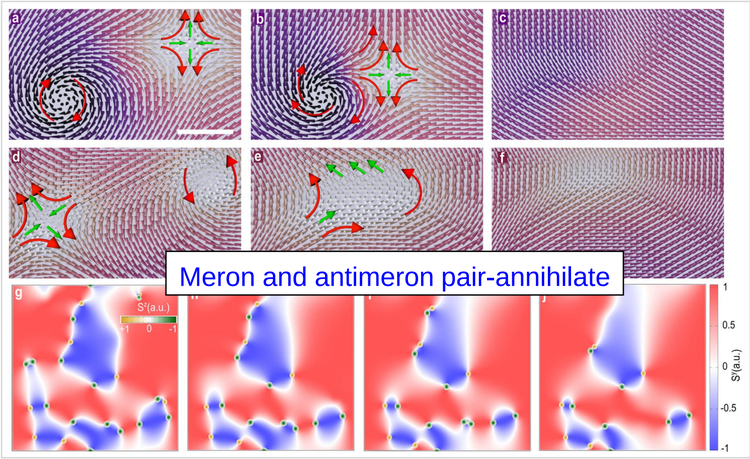
X.Z. Yu et al., Nature 564, 95 (2018)

Stable pairs via magnetic imprinting (Exp., Py thin film)



N. Gao et al., Nature Commun.,10, 5603 (2019)

Unstable pairs in 2D van der Waals magnet (Theo., $CrCl_3$)

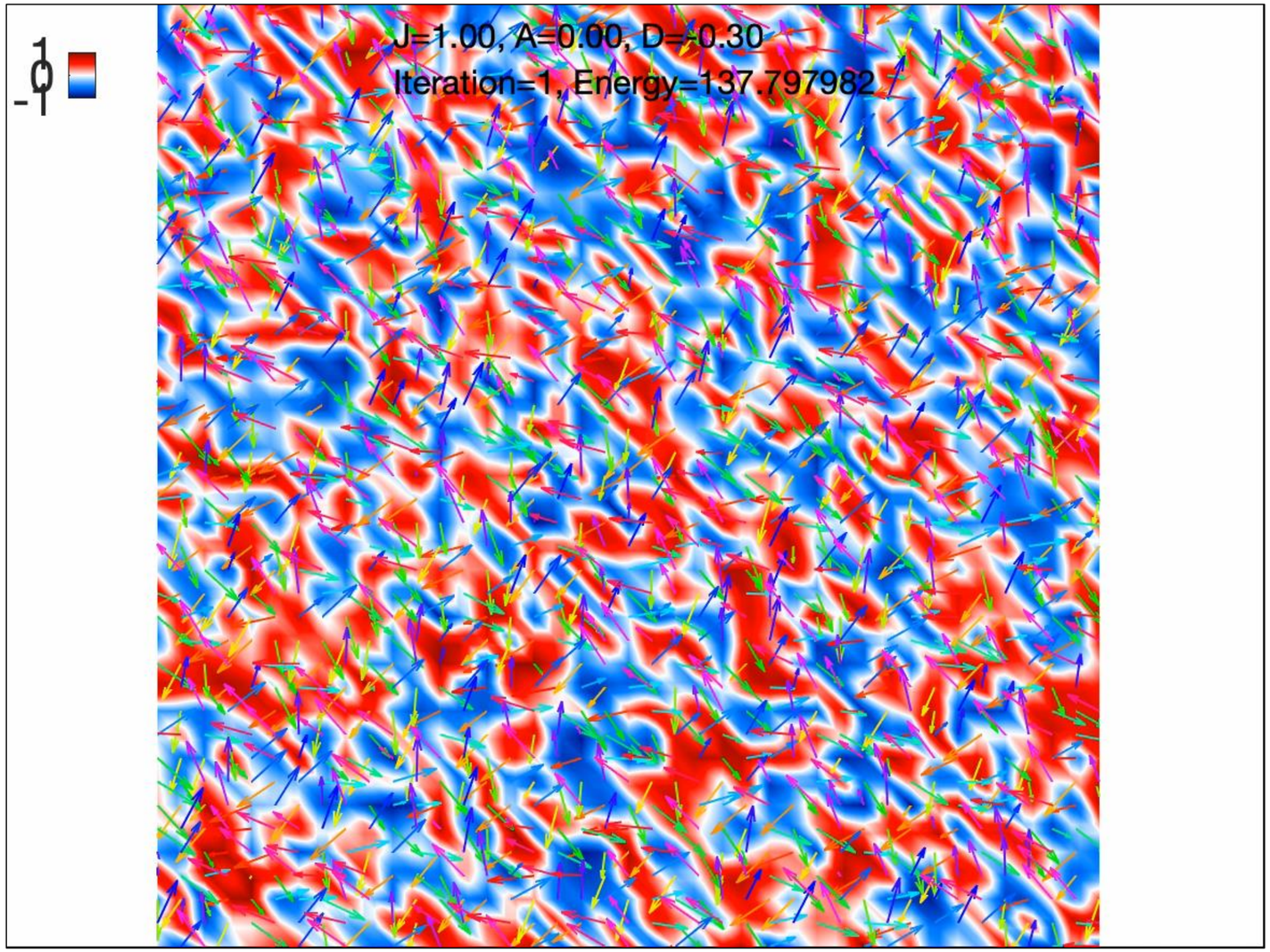


M. Augustin et al., Nat. Commun. 12, 185 (2021)

Unstable meron-antimeron pairs in conventional 2D magnets

- **Easy-plane ferromagnet**

$$\hat{H} = -\sum_{\langle i,j \rangle} J \boldsymbol{S}_i \cdot \boldsymbol{S}_j + D \sum_i S_i^z$$

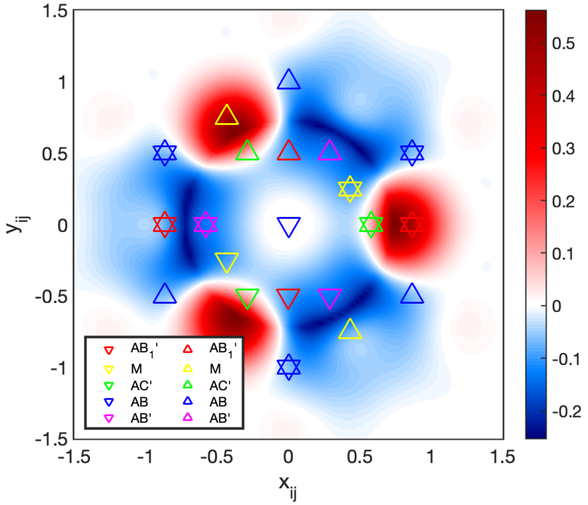


Moiré Magnets: Magnetic Domain Array Patterns

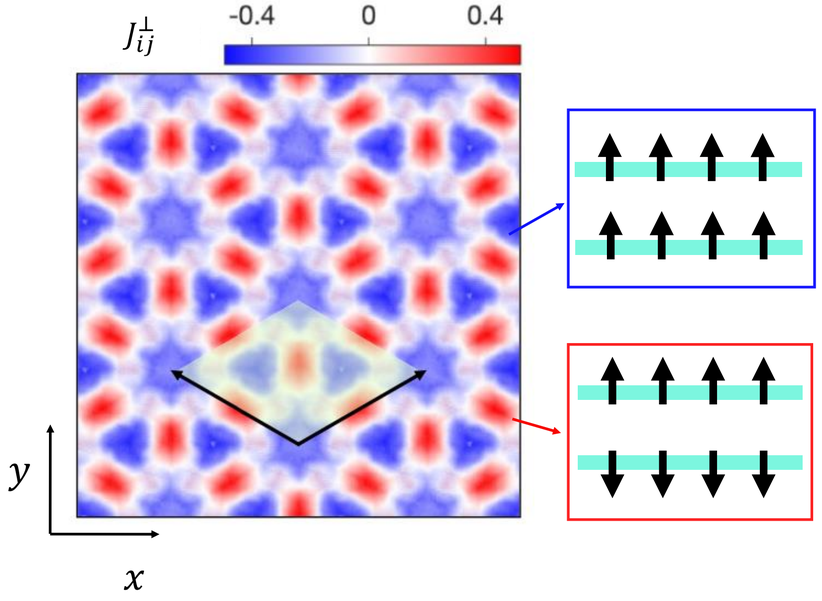
- Twisted bilayer easy-plane magnets

$$H = J \sum_{l=t,b} \sum_{\langle i,j \rangle} \mathbf{S}_i^l \cdot \mathbf{S}_j^l + A \sum_{l=t,b} \sum_i (\mathbf{S}_i^l \cdot \hat{\mathbf{z}})^2 + \sum_{i,j} J_{ij}^{\perp} \mathbf{S}_i^t \cdot \mathbf{S}_j^b$$

- **Ab-initio derived $J_{ij}^{\perp}$ (CrI$_3$)**

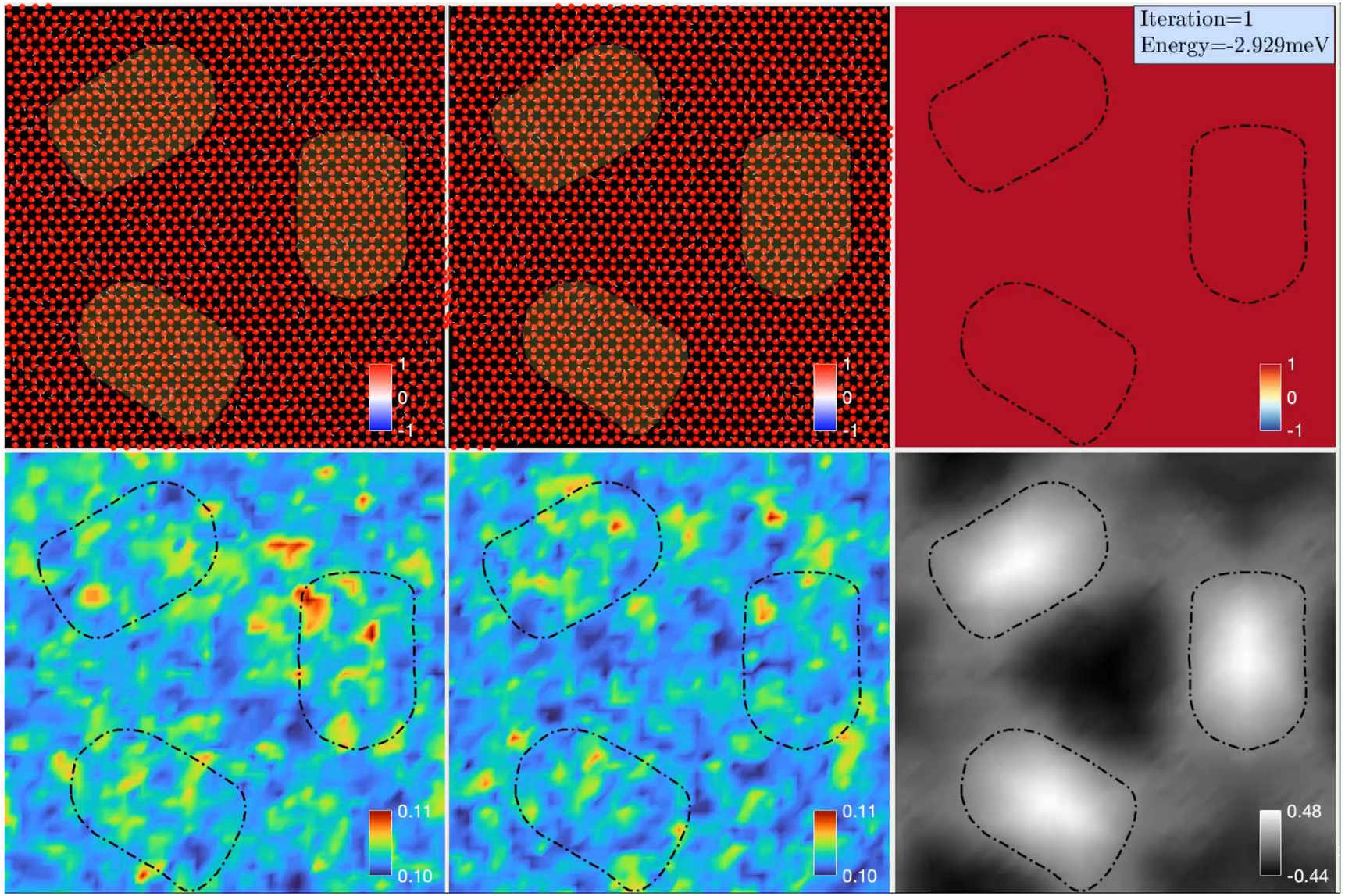


- Domain array patterns in twisted bilayer CrI3



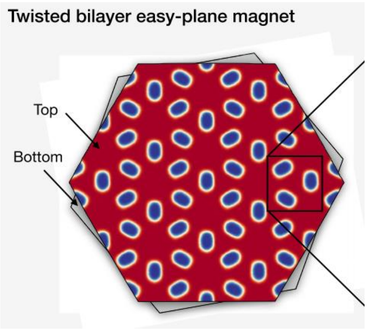
Using various domain array patterns, explore diverse potential topological soliton lattices.

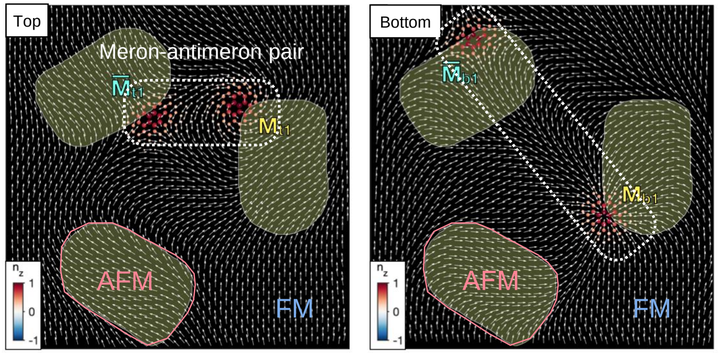
Stable meron-antimeron pairs in twisted magnets



Meron Quartet

- Domain array pattern → Meron lattice consisting of Meron Quartet





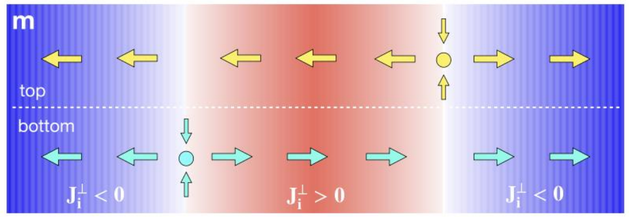
- **"Meron Quartet"** = Stable double meron-antimeron pairs

(1) One pair in each layer
(2) Meron and antimeron in each pair are separated by domains
(3) Each domain hosts two merons or antimerons

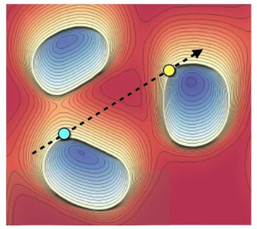
- **Crucial conditions** for generating stable meron-antimeron pairs

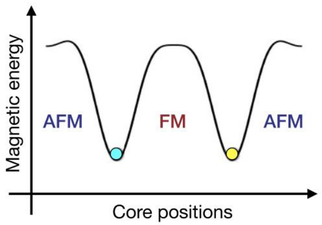
- Protection against pair annihilation

- Minimize interlayer exchange energy



- Energy barrier preventing core movements





Twisted bilayer easy-plane ferromagnets can create a meron lattice with a unique Meron Quartet configuration.

Nano Lett. 2024, 24, 1, 74–81

Outline

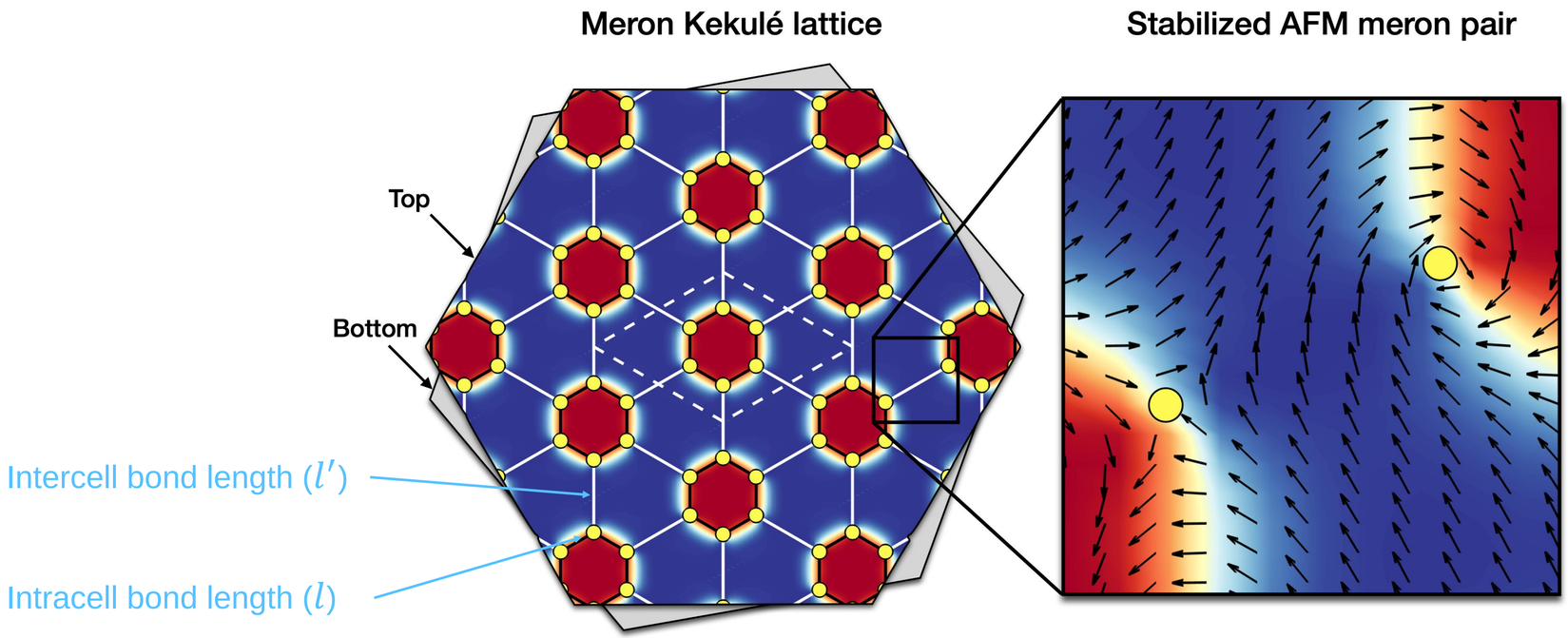
I. Twist Engineering of 2D Magnetism

II. Meron Kekulé Lattices in Twisted Antiferromagnets

npj Quantum Materials 10, 68, (2025)

Meron Kekulé lattices in in twisted vdW antiferromagnets

- Meron lattices in twisted bilayer easy-plane Neél antiferromagnets



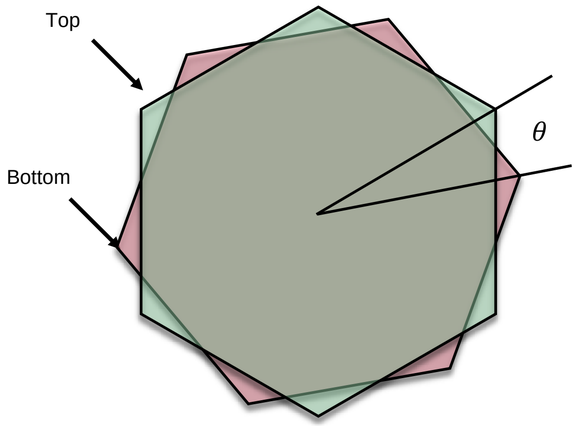
Yellow Dots = Meron Cores

Arrows = Neél vectors

$$\boldsymbol{N}_i^{t,b} = \frac{\boldsymbol{S}_{i,A}^{t,b} - \boldsymbol{S}_{i,B}^{t,b}}{\left|\boldsymbol{S}_{i,A}^{t,b} - \boldsymbol{S}_{i,B}^{t,b}\right|}.$$

- Meron Kekulé lattice = a distorted arrangement of meron cores ($l \neq l'$)

Spin model for a twisted bilayer Néel antiferromagnet



- AFM intralayer exchange + easy-plane single-ion anisotropy

$$H_{intra} = J \sum_{l=t,b} \sum_{\langle i,j \rangle} \mathbf{S}_i^l \cdot \mathbf{S}_j^l + A \sum_{l=t,b} \sum_i (\mathbf{S}_i^l \cdot \hat{\mathbf{z}})^2$$

$J = 1$ meV, $A = 0.2$ meV

- Interlayer AFM exchange coupling

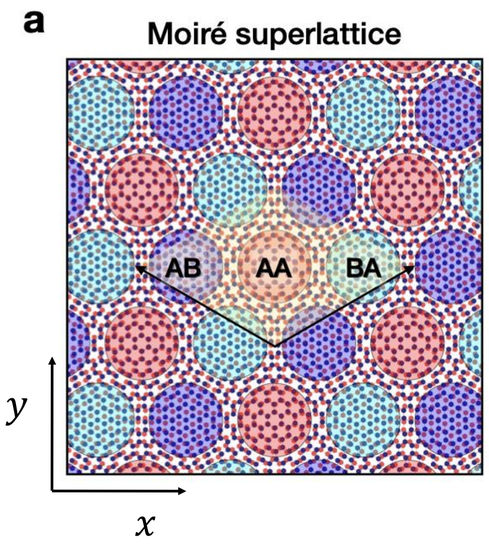
$$H_{inter} = \sum_{i,j} J_{ij}^{\perp} \mathbf{S}_i^t \cdot \mathbf{S}_j^b$$

where $J_{ij}^{\perp} = J_0^{\perp} \exp[-\alpha(|\mathbf{r}_{ij}^{tb}|/d - 1)]$ with $|\mathbf{r}_{ij}^{tb}| = \sqrt{|\mathbf{r}_{ij}^{\parallel}|^2 + d^2}$

$J_0^{\perp} = 0.3$ meV, $\alpha = 15$, $d/a = 1.75$

Moiré-patterned interlayer coupling

- Structural modulation

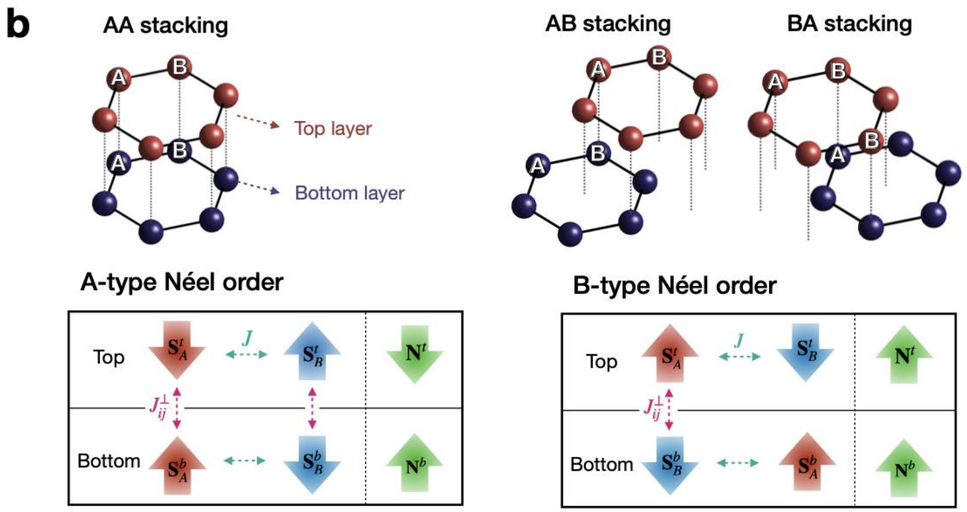


AA stacking

AB stacking

BA stacking

- Emergence of two Néel orders



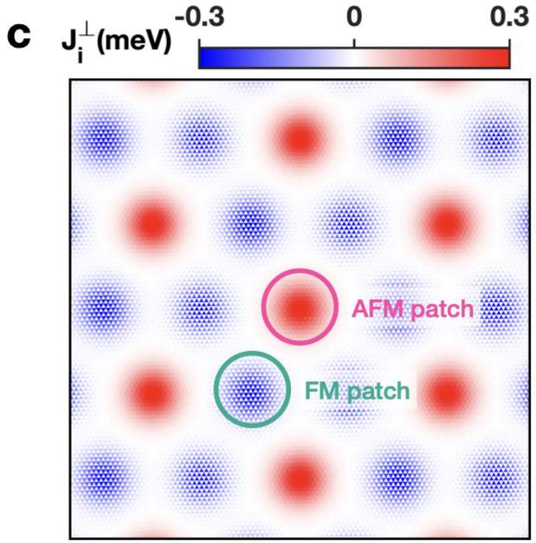
Néel vectors:

$$|\mathbf{N}_i^l| = \frac{\mathbf{S}_{i,A}^l - \mathbf{S}_{i,B}^l}{|\mathbf{S}_{i,A}^l - \mathbf{S}_{i,B}^l|}$$

A-type Néel order: $\mathbf{N}_i^t \cdot \mathbf{N}_i^b = -1$

B-type Néel order: $\mathbf{N}_i^t \cdot \mathbf{N}_i^b = +1$

- Patterned interlayer exchange

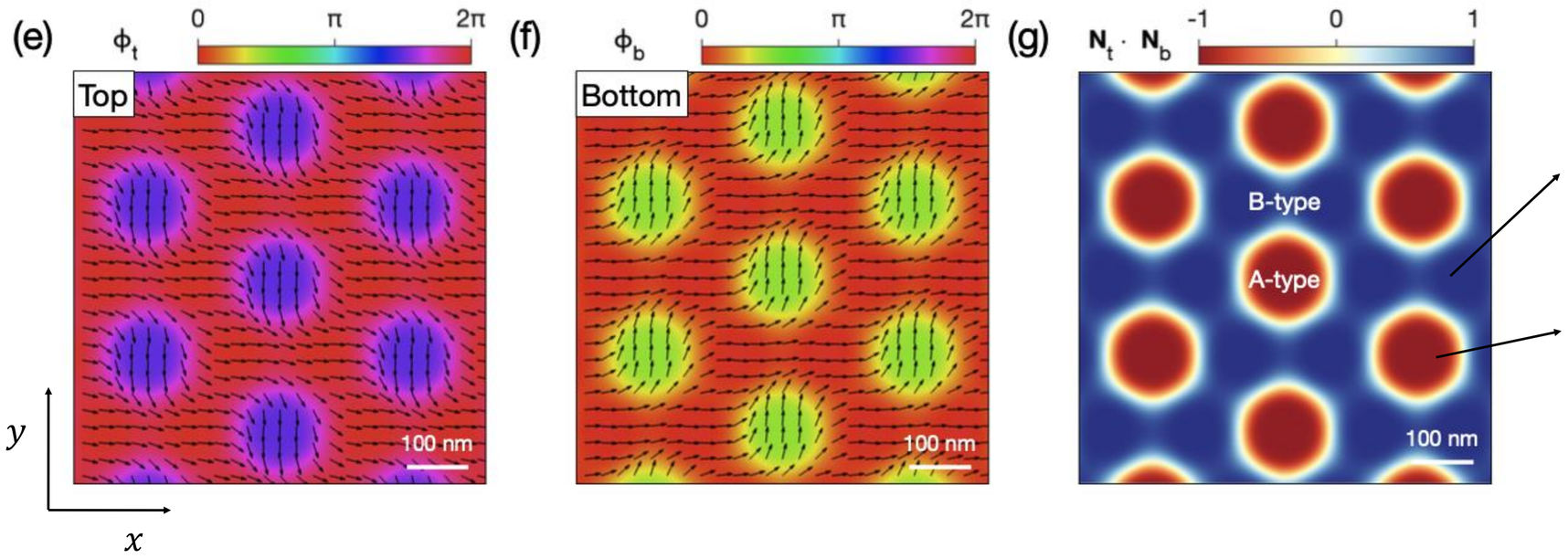


Red: A-type Néel

Blue: B-type Néel

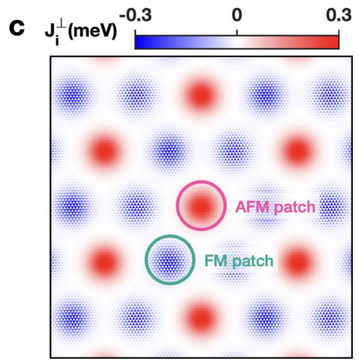
Magnetic ground state

- Magnetic domain array: Periodic domain structure showing both A-type and B-type Néel orders



Parallel alignment between $\mathbf{N}_i^t$ and $\mathbf{N}_i^b$

Antiparallel alignment between $\mathbf{N}_i^t$ and $\mathbf{N}_i^b$



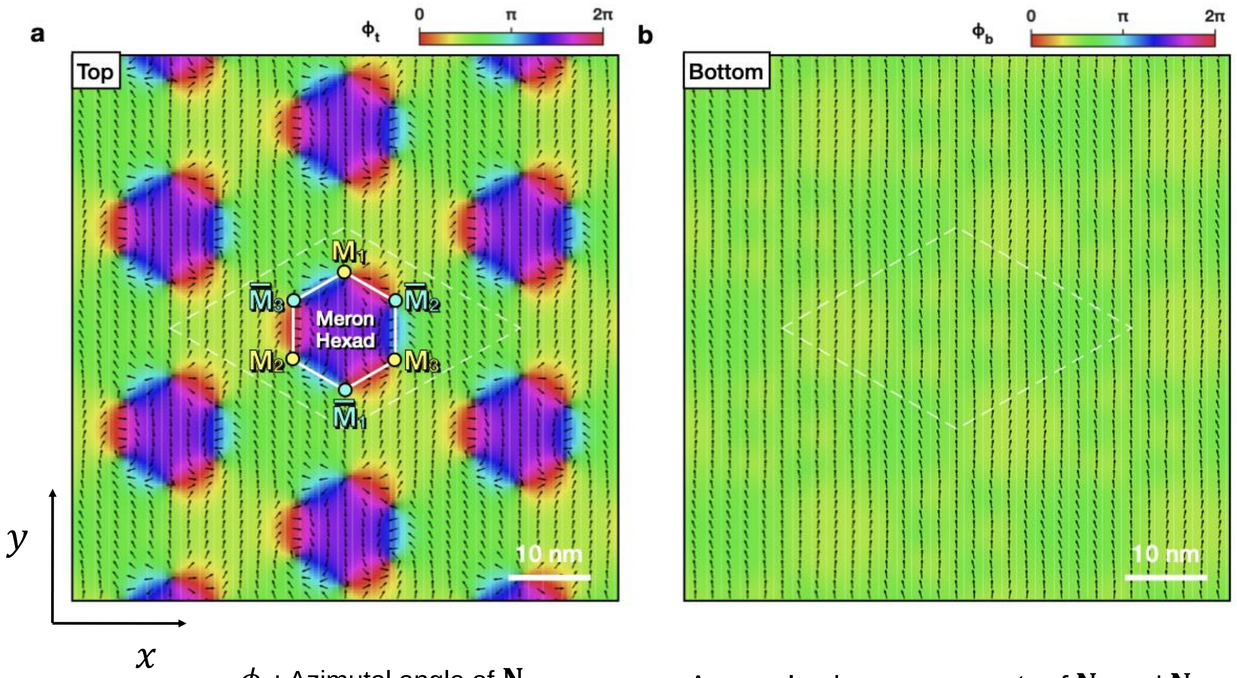
- $\mathbf{N}_t$: Néel order on the top layer
- $\mathbf{N}_b$: Néel order on the bottom layer

- ϕ_t: Azimutal angle of $\mathbf{N}_t$
- ϕ_b: Azimutal angle of $\mathbf{N}_b$
- Arrows: In-plane components of $\mathbf{N}_t$ and $\mathbf{N}_b$

- Red: $\mathbf{N}_t \cdot \mathbf{N}_b = -1$ (A-type Néel order)
- Blue: $\mathbf{N}_t \cdot \mathbf{N}_b = +1$ (B-type Néel order)
- Minimizes the interlayer exchange energy

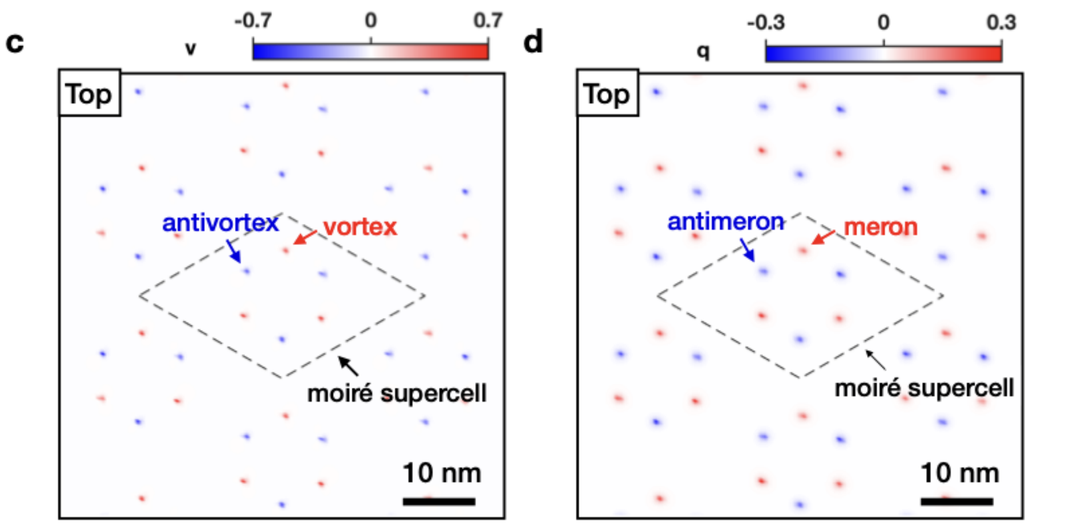
Metastable meron state

- A meron lattice: Periodic arrangement of meron and antimeron cores



- ϕ_t: Azimutal angle of $\mathbf{N}_t$
- ϕ_b: Azimutal angle of $\mathbf{N}_b$

- Arrows: In-plane components of $\mathbf{N}_t$ and $\mathbf{N}_b$
- Black colors -> Meron cores



$$v(x,y) = \frac{1}{\pi}\hat{\boldsymbol{z}} \cdot (\partial_x \boldsymbol{N}(x,y) \times \partial_y \boldsymbol{N}(x,y))$$

$$q(x,y) = \frac{1}{4\pi}\boldsymbol{N}(x,y) \cdot (\partial_x \boldsymbol{N}(x,y) \times \partial_y \boldsymbol{N}(x,y)),$$

- $w = +1$ for $\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$
- $w = -1$ for $\overline{\mathbf{M}}_1, \overline{\mathbf{M}}_2, \overline{\mathbf{M}}_3$

- $Q = -\frac{1}{2}$ for $\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$
- $Q = \frac{1}{2}$ for $\overline{\mathbf{M}}_1, \overline{\mathbf{M}}_2, \overline{\mathbf{M}}_3$

- **Top layer**

  - Three vortices: $\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$
  - Three antivortices: $\overline{\mathbf{M}}_1, \overline{\mathbf{M}}_2, \overline{\mathbf{M}}_3$

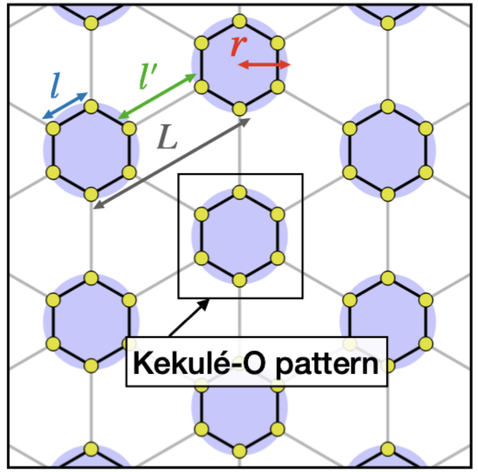
- **Bottom layer**

  - Uniform Néel order

- **Three merons ($\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$):** $Q = -\frac{1}{2}, w = +1, p = \frac{1}{2}$
- **Three antimerons ($\overline{\mathbf{M}}_1, \overline{\mathbf{M}}_2, \overline{\mathbf{M}}_3$):** $Q = +\frac{1}{2}, w = -1, p = \frac{1}{2}$

“Meron Kekulé lattice”

a Meron Kekulé lattice

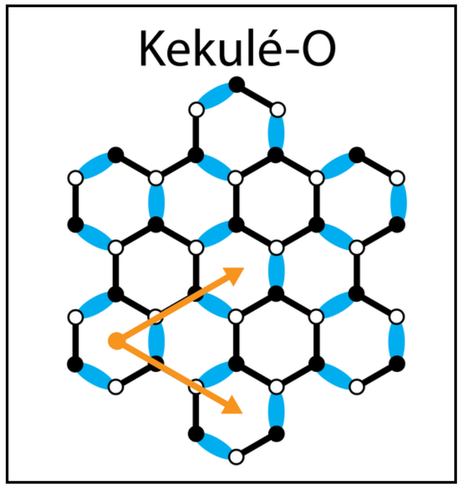


- Intracell bond length (l)
- Intercell bond length (l')
- Superlattice periodicity$(L = 2l - l')$

If $l \neq l'$, the meron lattice becomes a honeycomb lattice

However, $l \neq l'$, since they are determined by energetic balance between $J_{ij}^{\perp}$ and J

Kekulé lattice: a non-regular lattice structure with distortion



https://www.fkf.mpg.de/

Kekulé-O structure: a distorted honecomb lattice with $l \neq l'$

- Kekulé lattices in graphene

  Nat. Phys. 12, 950 (2016)

- Kekulé lattices in phononic and photonic crystal structures

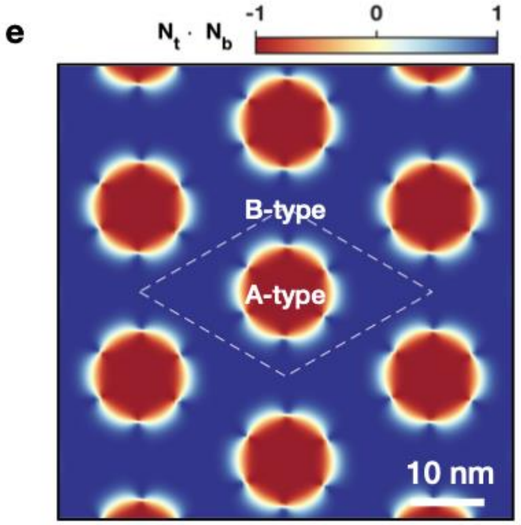
  Photon. Res. 10, 999 (2022)

  Phys. Rev. Appl. 11, 044086 (2019)

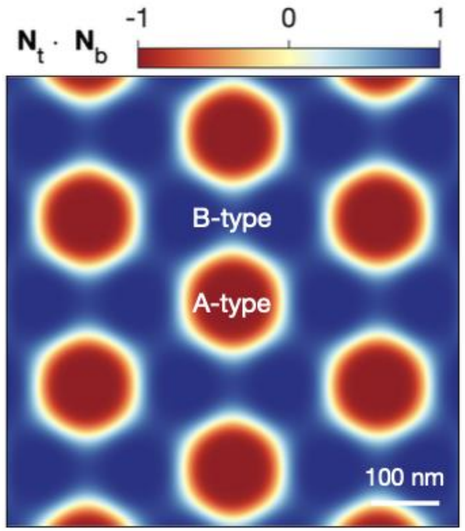
- First example of a Kekulé lattice composed of topological solitons (merons)

Stabilization mechanism of the Meron Kekulé lattice

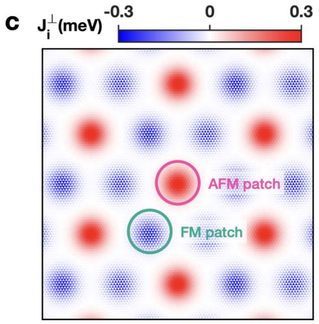
- Meron Kekulé lattice miminizes the interlayer exchange

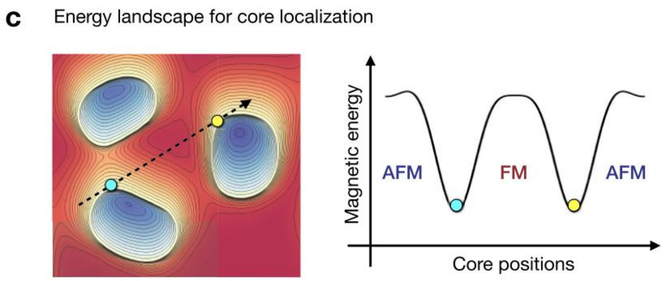


- Meron Kekulé lattice



- Ground state

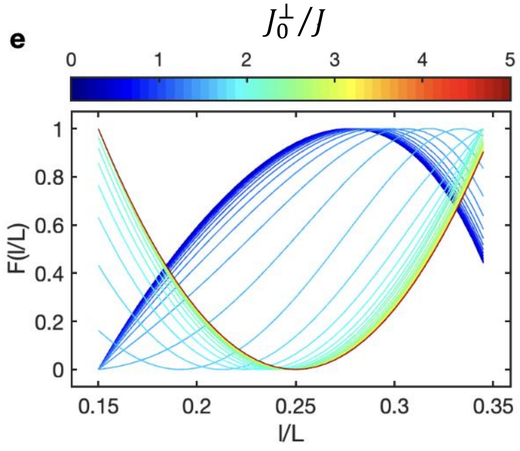




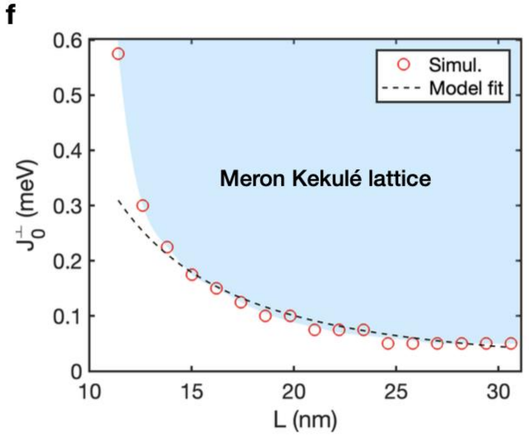
KM Kim et al., Nano Lett., 24, 1, 74–81 (2024)

- Effective Moiré potential for localizing meron cores

$$E(l) = C_1 J \ln\left[\sqrt{\frac{2l}{3L}}\frac{\left(L^6 - l^6\right)^2\left(L^6 - 64l^6\right)}{L^6\left(L^6 + 27l^6\right)^2}\right] + \frac{C_2 J_0^{\perp}}{a^2}(l - r)^2.$$



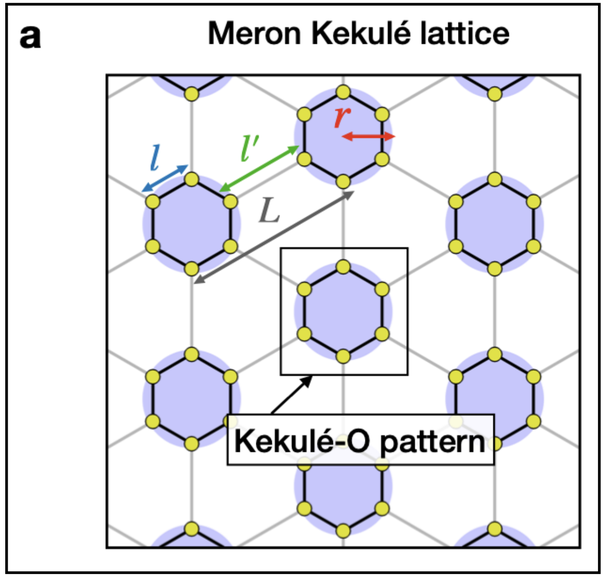
- "Potential well" for meron cores



- Stabilization at large L or $J_0^{\perp}$

Tunability of the Kekulé structure

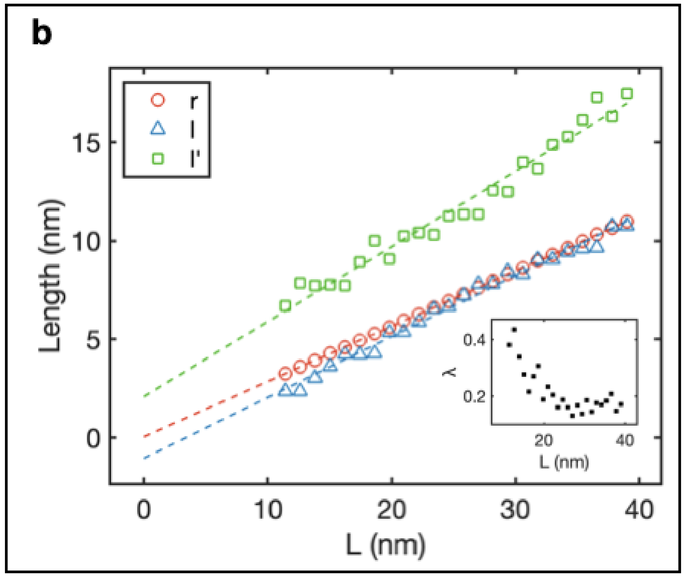
- Manipulation of Kekulé structure



Stabilization condition → $r \approx l$

Adjusting r → Manipulation of l

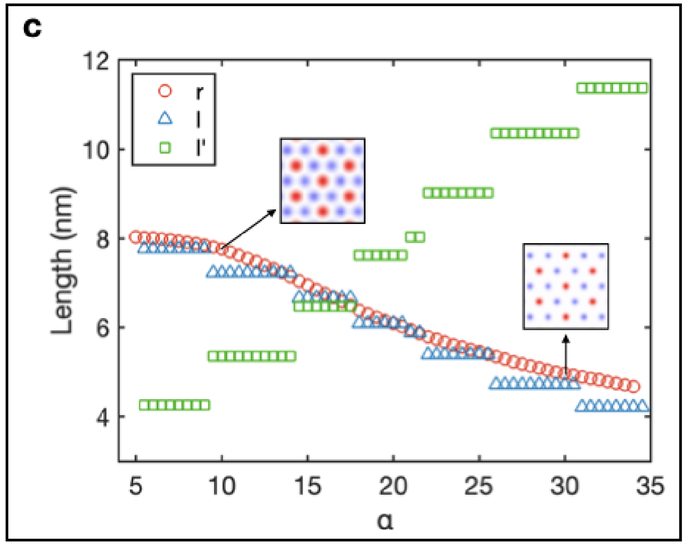
- By adjusting L



Increase of L → Increase of r

Increase of r → Increase of l

- By adjusting α



Increase of α → Decrease of r

Decrease of r → Decrease of l

Diverse meron lattice configurations

- **SO(2) spin rotational symmetry in the x-y plane**

Free helicity: $\phi_i^t \rightarrow \phi_i^t + \phi_0$

- **Z2 spin symmetry in the z axis**

Free polarity: $p = \pm\frac{1}{2}$ for each meron core

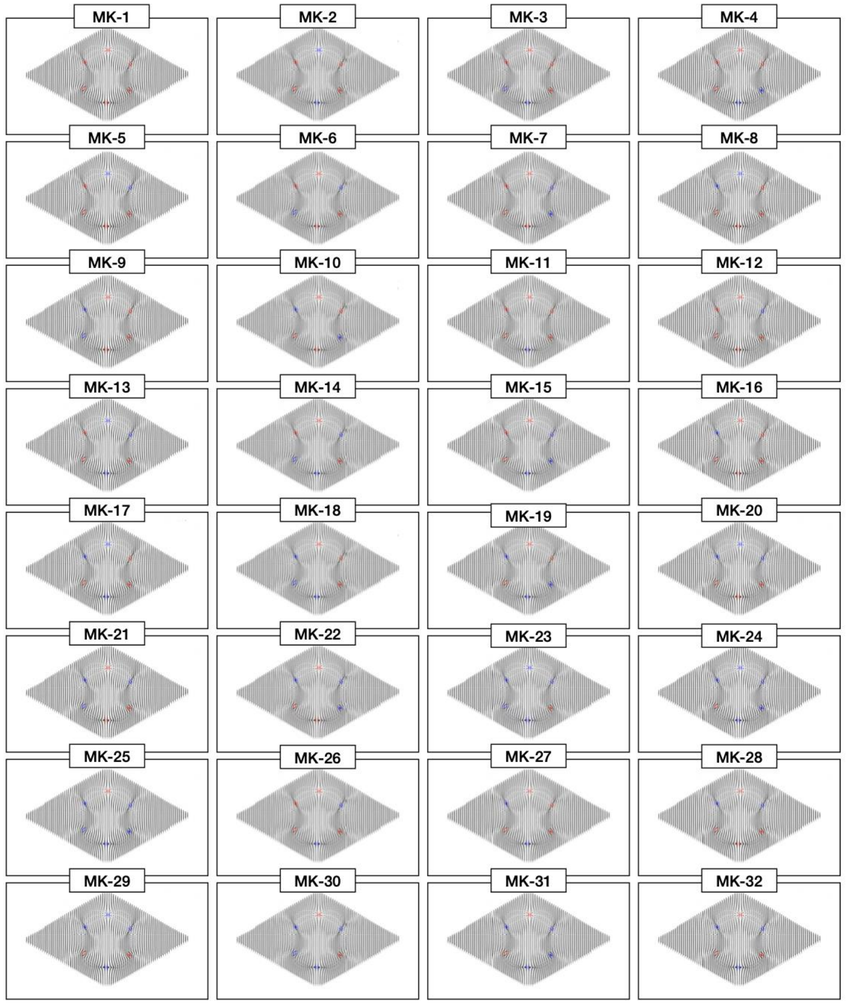
$$\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \overline{\mathbf{M}}_1, \overline{\mathbf{M}}_2, \overline{\mathbf{M}}_3$$

- 32 Meron Kekule lattice structures in total

- Show minimal energy variations (difference less than 0.003%)

- 6 merons $(Q_{tot} = -3)$, 5 merons + 1 antimeron $(Q_{tot} = -2)$, $\cdots$, 6 antimerons $(Q_{tot} = +3)$

32 distinct Meron Kekulé lattices

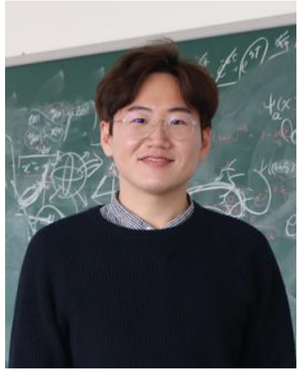


Summary

- Moiré-patterned interlayer coupling → Stabilization of meron-antimeron pairs
- Meron Kekulé lattice = Distorted honeycomb lattice of meron cores
- Effective Moiré potential for meron cores as a stabilization mechanism
- Tunability of the lattice structure
- Polarity and helicity degrees of freedom, and different skyrmion numbers

Acknowledgements

Prof. Se Kwon Kim
(KAIST)



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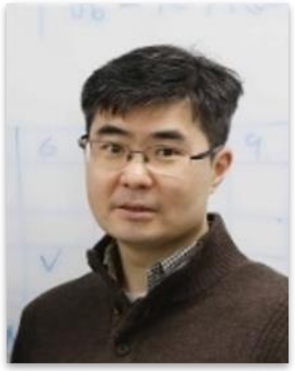

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Thank you for your attention!