Stacking Domain Wall Magnons in Twisted van der Waals Magnets

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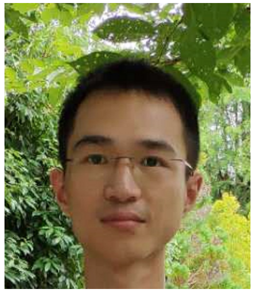

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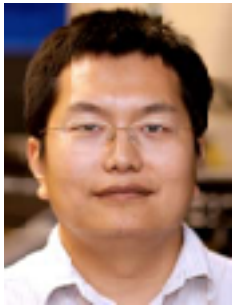

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PERSPECTIVE

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Van der Waals heterostructures

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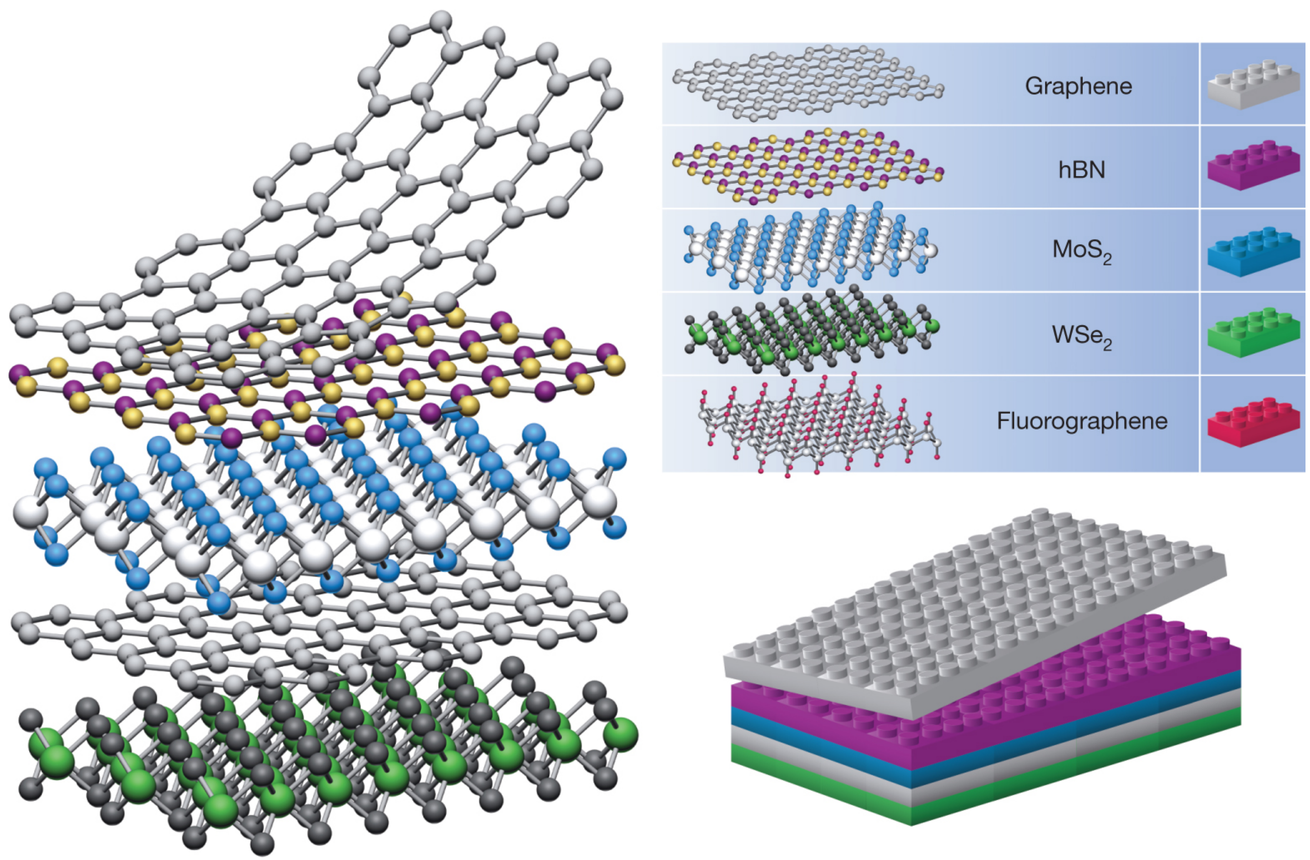
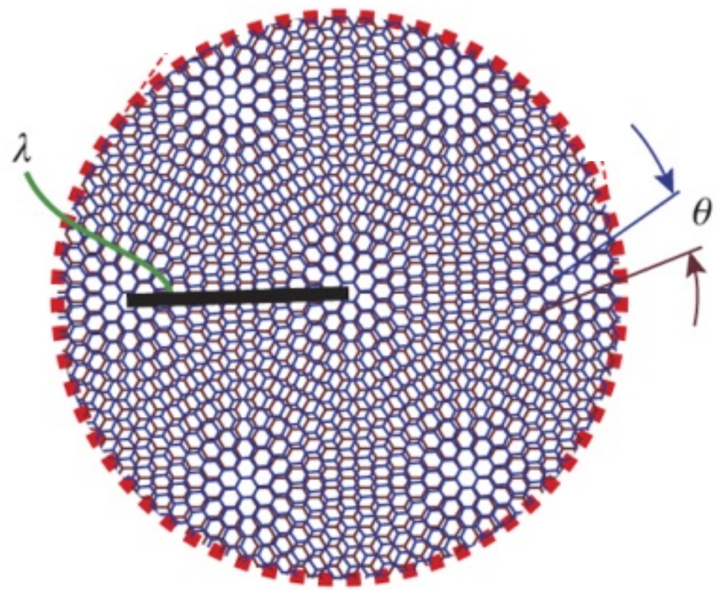
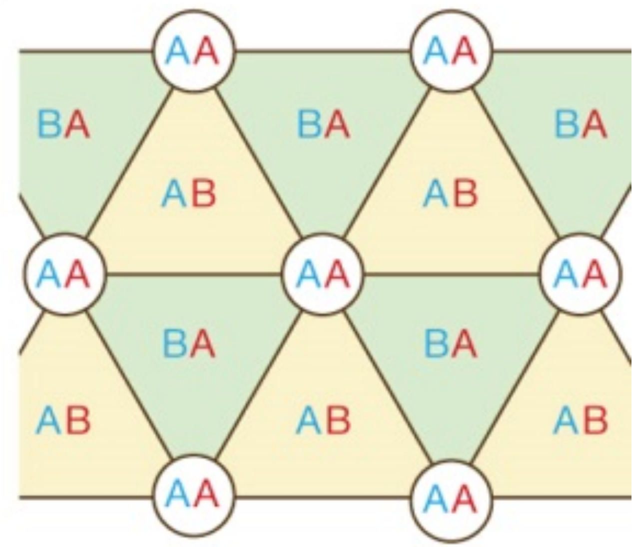


Stacking engineering

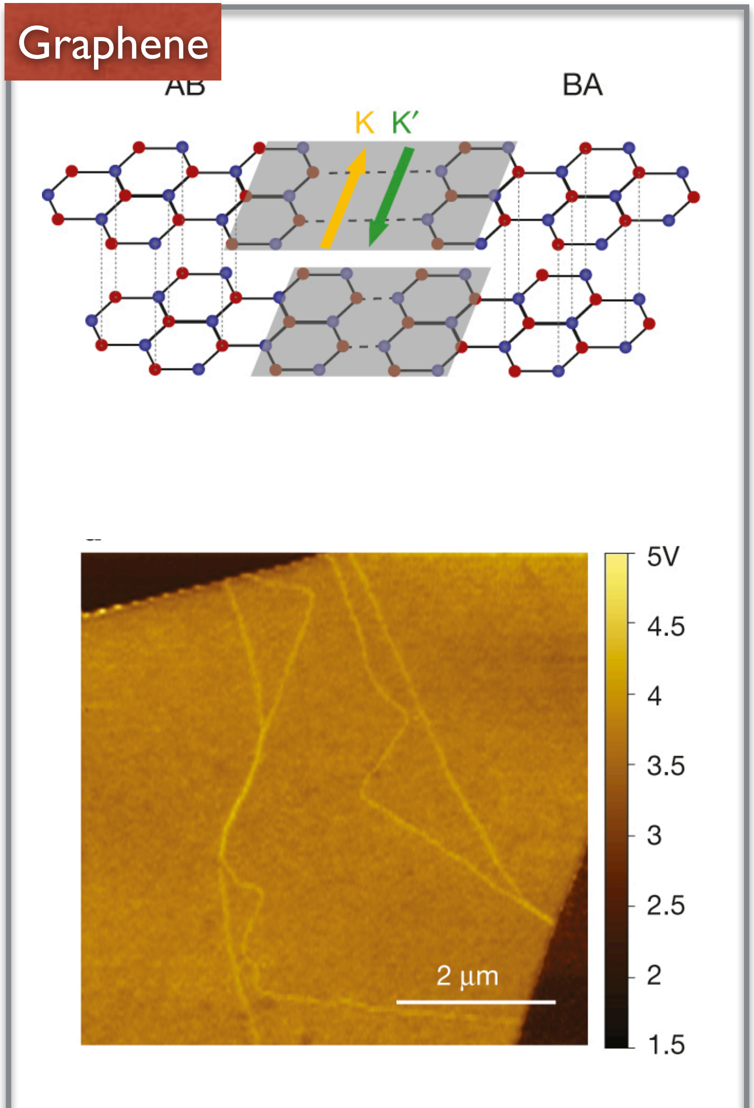




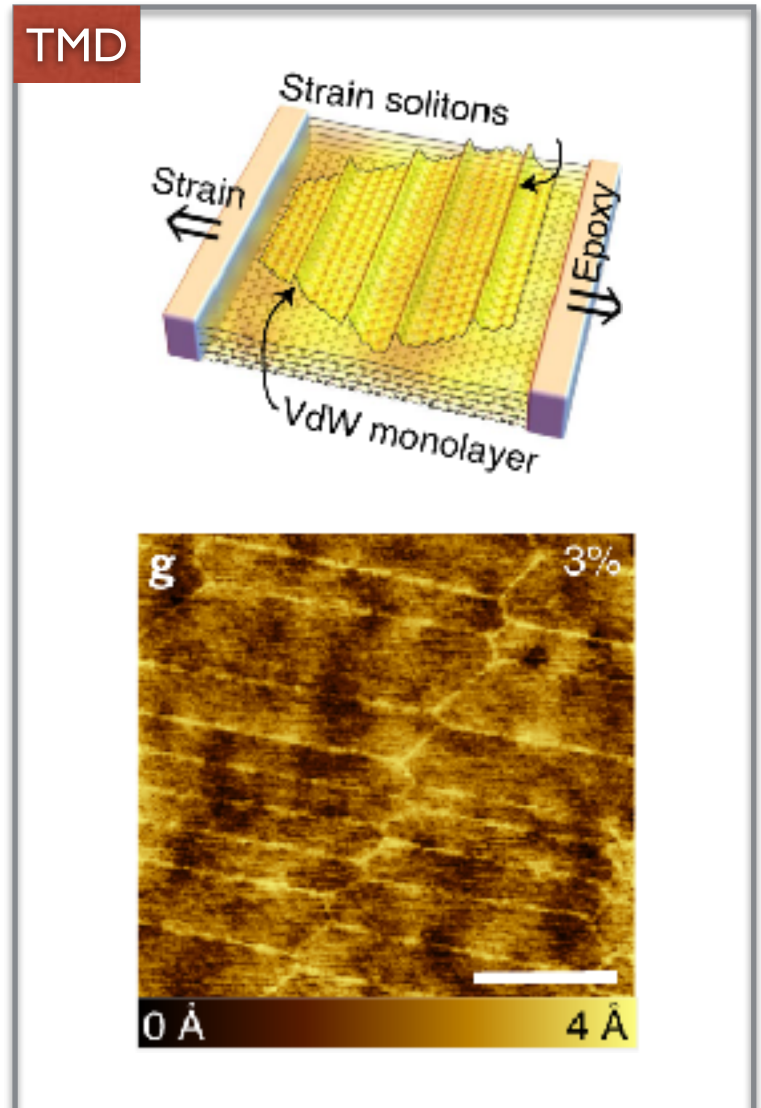
Cao… Jarillo-Herrero (2018)

Twistronics fundamentally is stacking engineering

Stacking DWs are ubiquitous

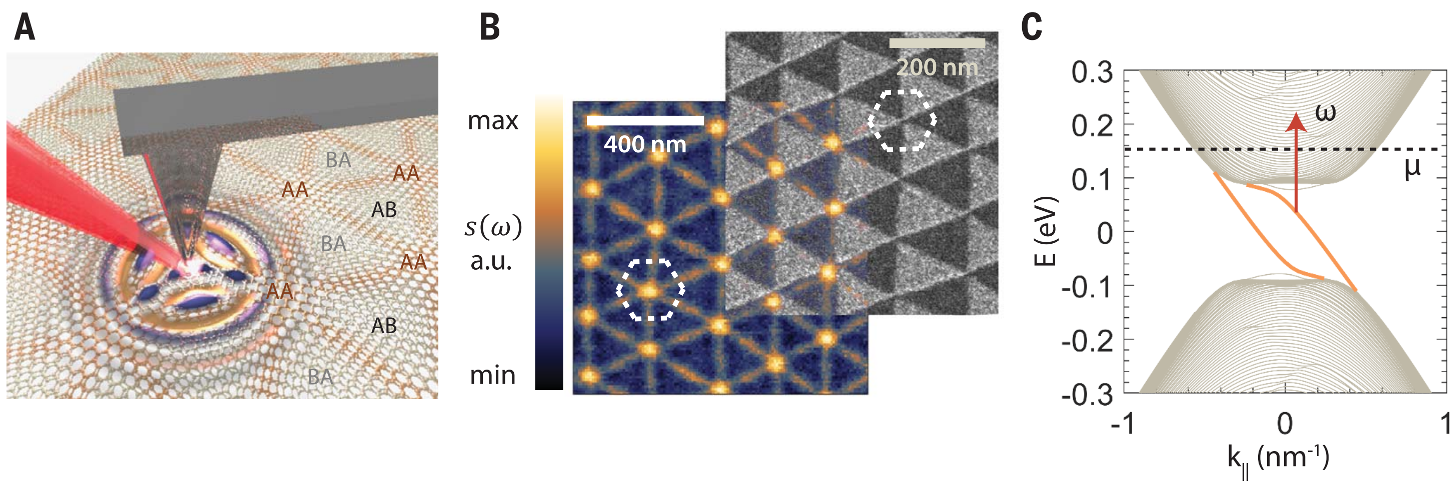


Ju… Wang, Nature (2015)



Edelberg…Ochoa, Pasupathy, Nat. Phys. (2020)

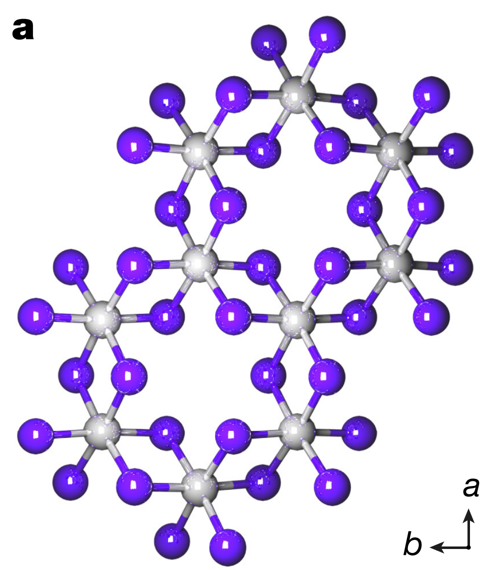
1D confined channels

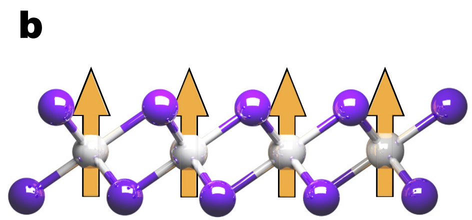


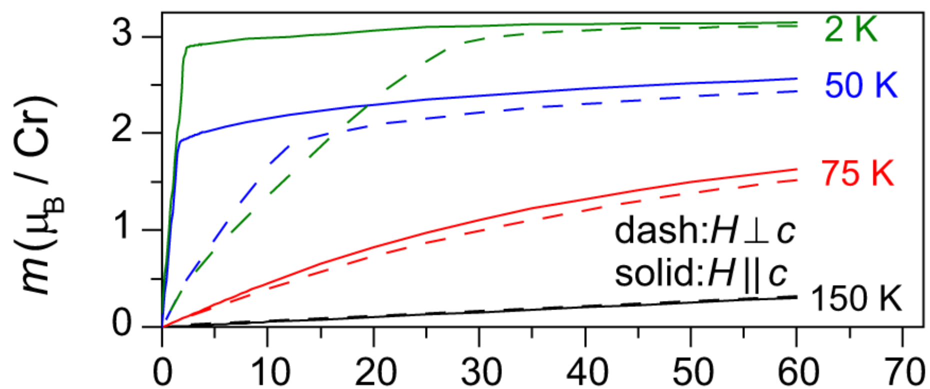
Sunku…Basov, Science (2018)

What about 2D magnets?

CrI_3: a prototypical 2D magnet



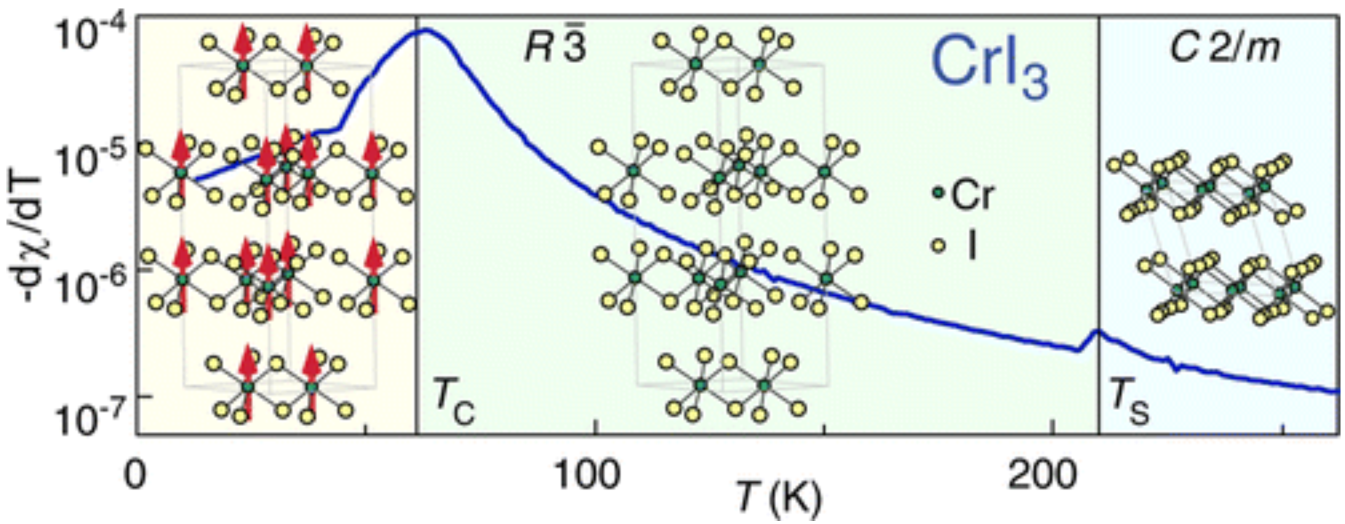




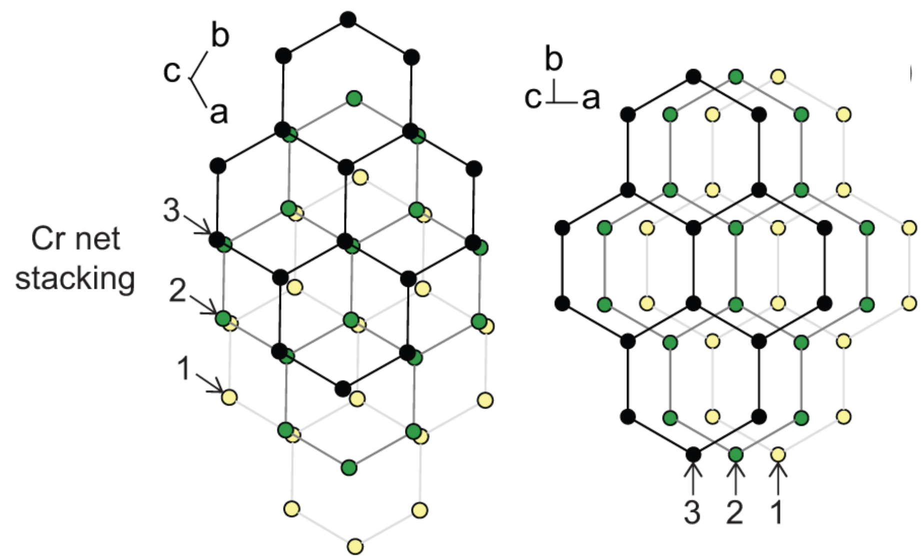
CrI_3 is a bulk ferromagnet with a strong out-of-plane easy axis

McGuire et al, Chem. Mater. **27**, 612 (2015)

Structural phase transition

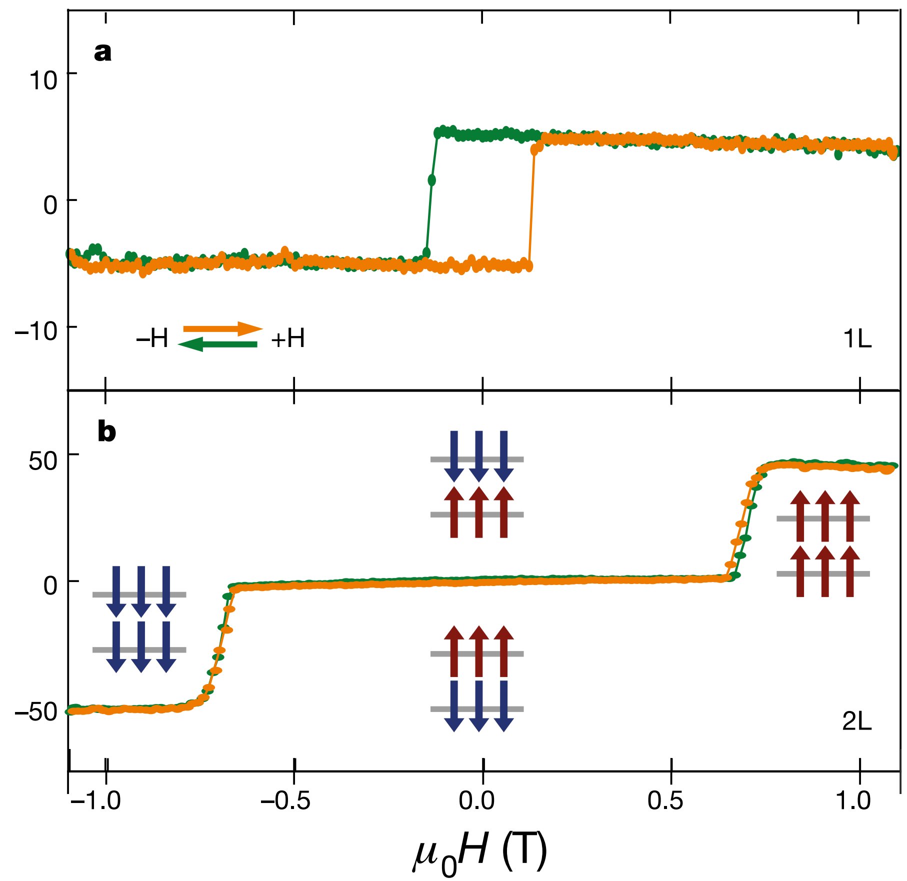


CrI₃ undergoes a structural phase transition from monoclinic to rhombohedral at around 210 K



McGuire et al, Chem. Mater. **27**, 612 (2015)

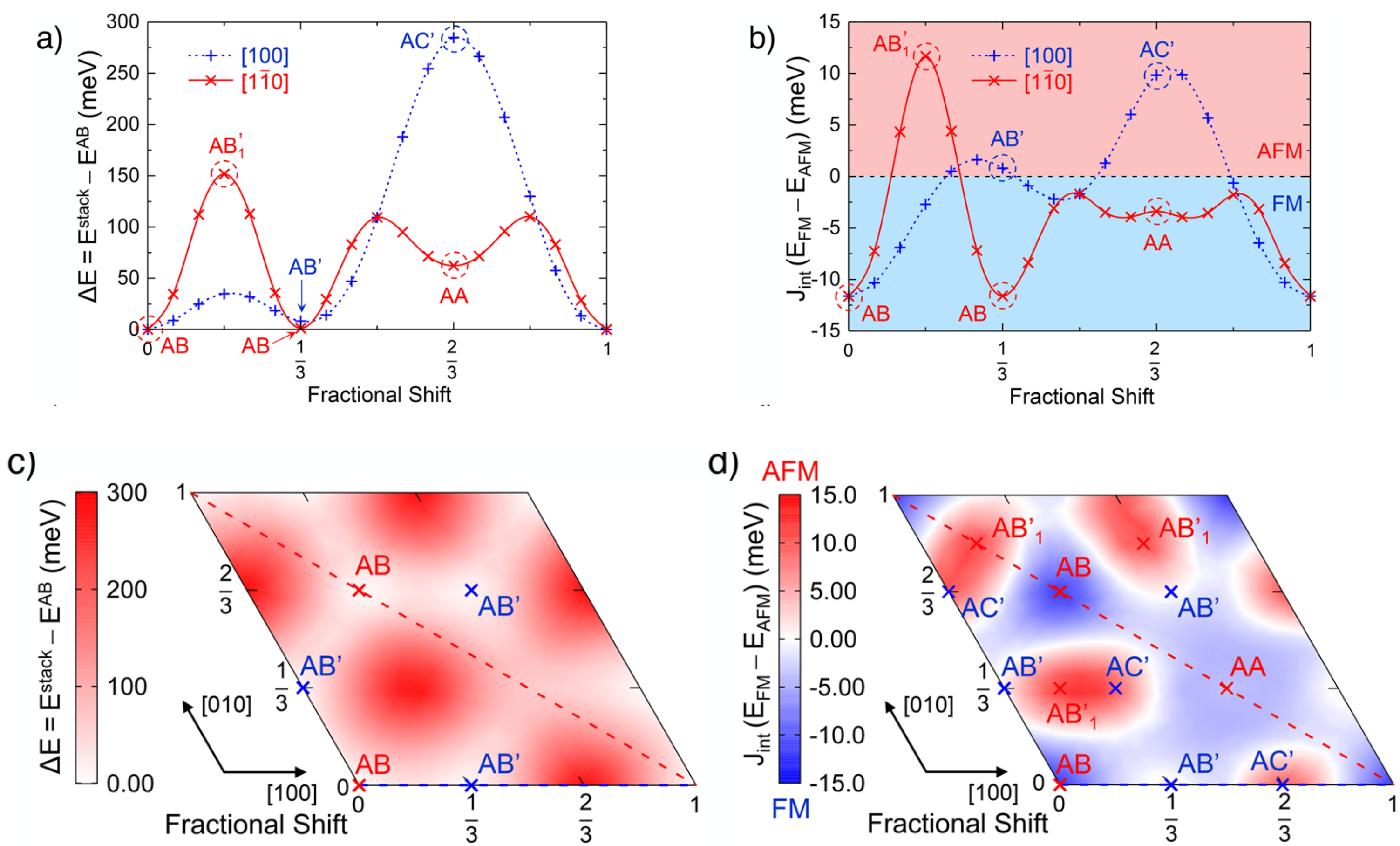
Atomically thin CrI_3



CrI3 is a FM in bulk, but AF for thin flakes. Why?

Huang, DX, Jarillo-Herrero, Xu et al, Nature (2017)

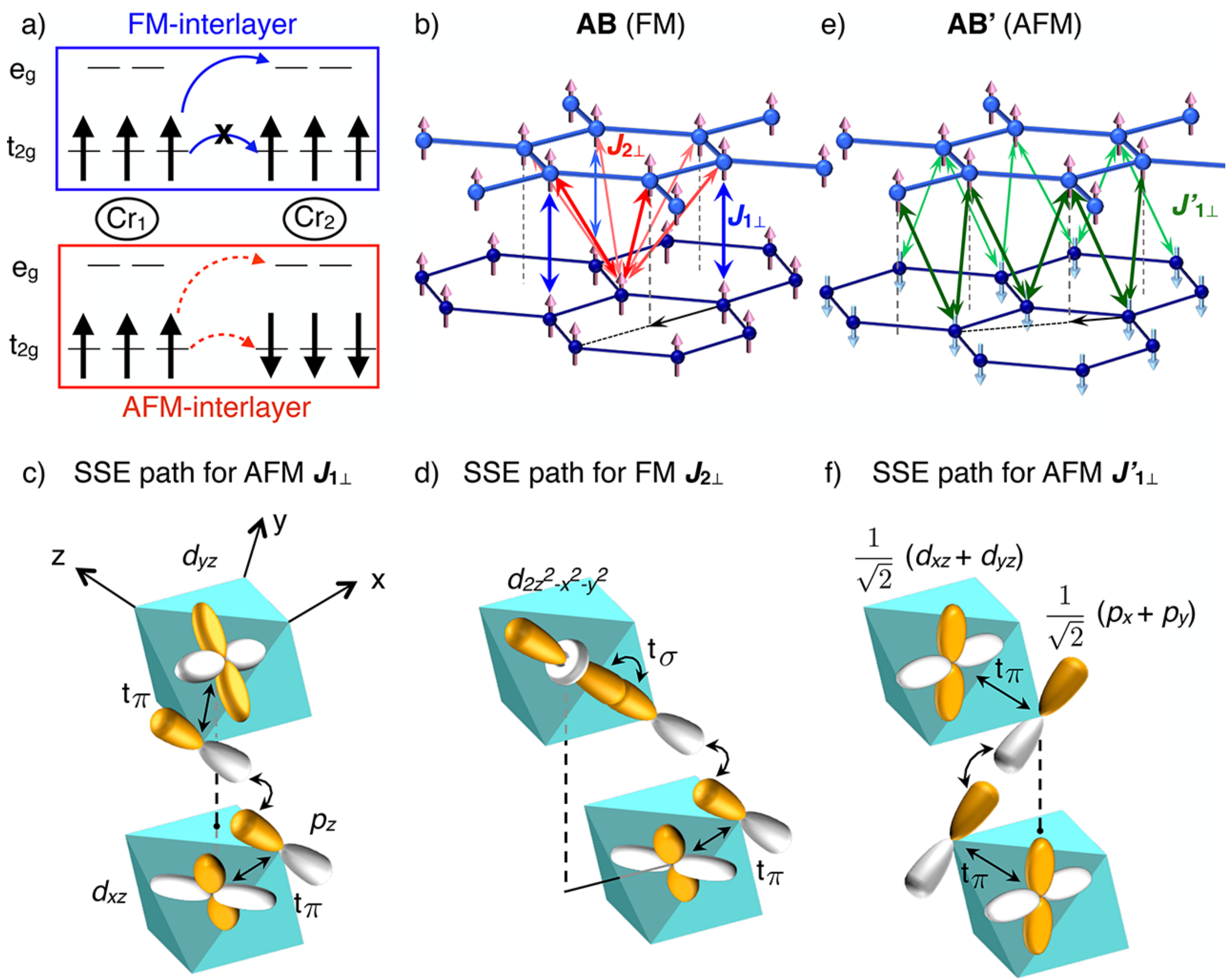
Stacking and magnetic energy



rhombohedral (AB) ⇒ FM Monoclinic (AB') ⇒ AFM

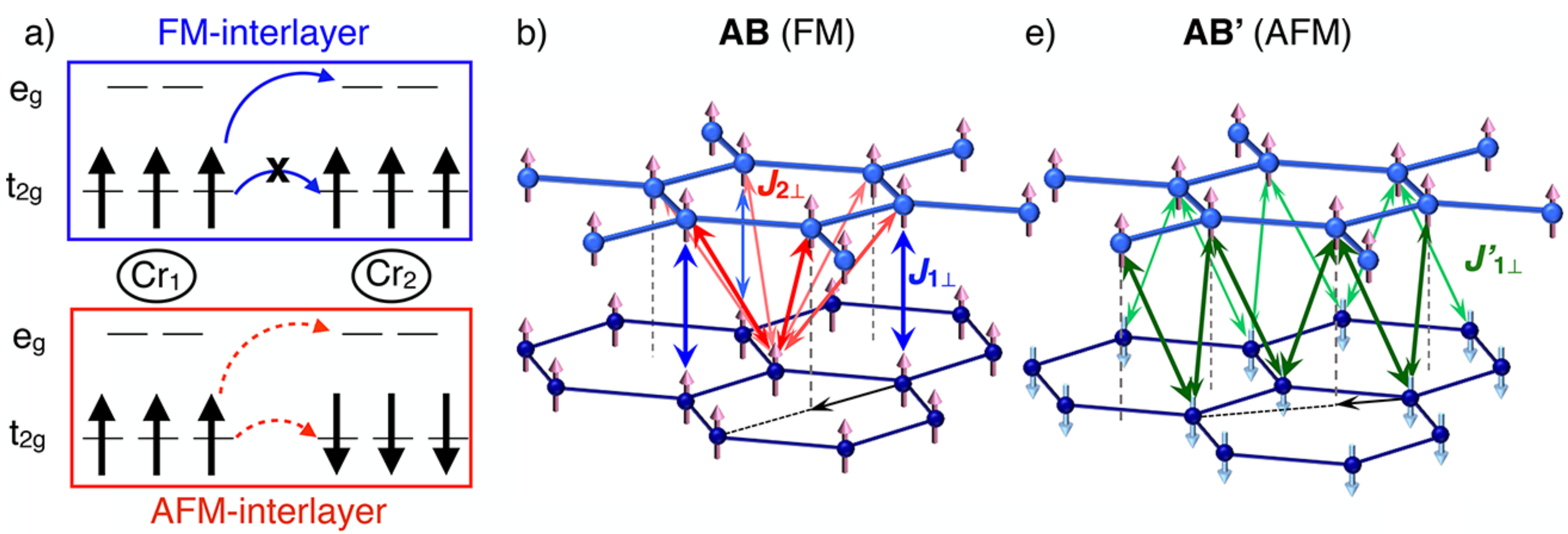
Sivadas, Okamoto, Xu, Fennie, DX Nano Lett. **18**, 7658 (2018)

Interlayer super-super exchange



Interlayer super-super exchange

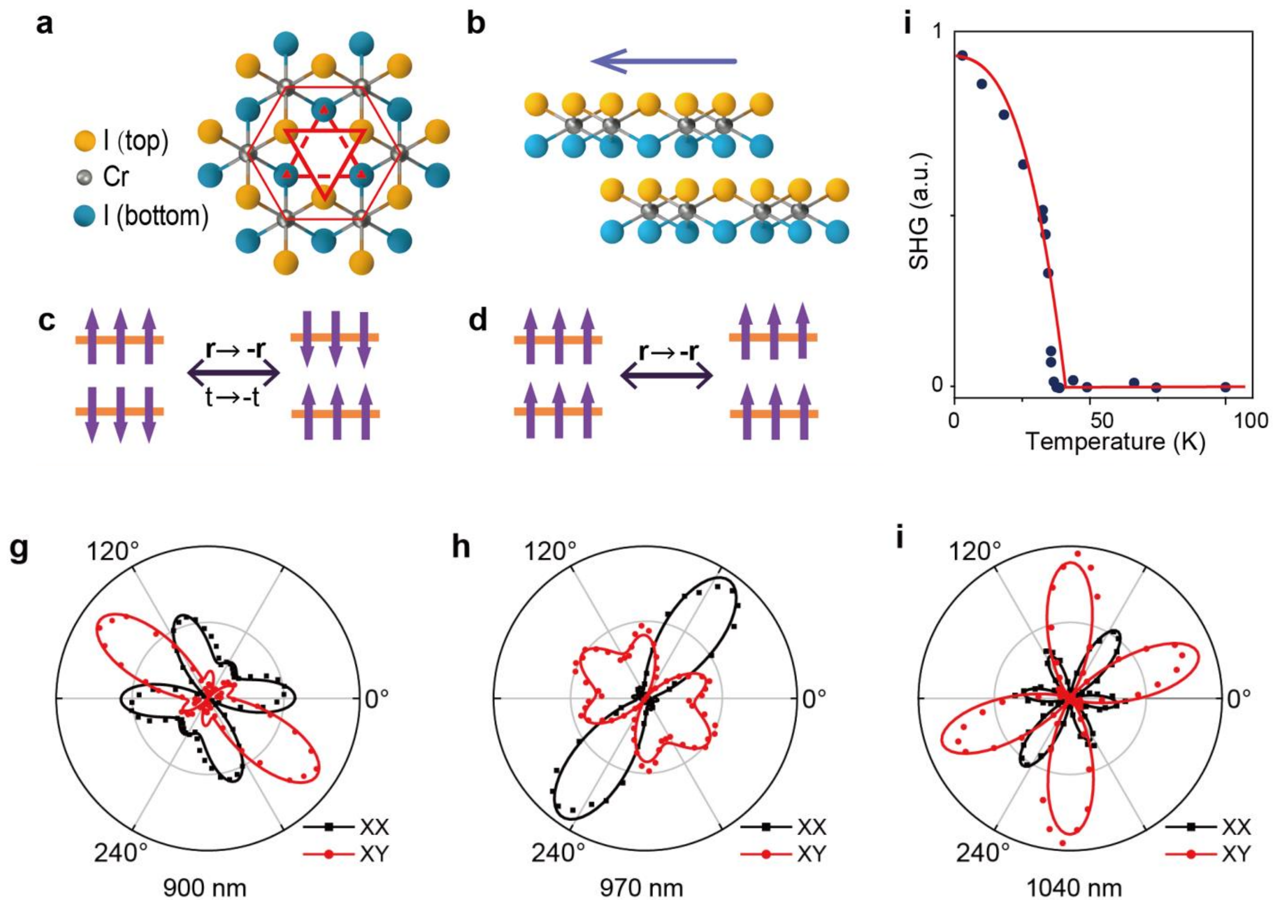
Stacking	Cr–Cr NN (Å)	Cr–Cr second-NN (Å)	I–I (Å)
AB	6.7 (6.7) [1]	7.8 (7.8) [16]	4.2 (4.2)
AB′	7.1 (7.1) [6]	8.1 (8.2) [6]	4.2 (4.2)



Stacking dependent magnetism is tied to local stacking of octahedrons.
Applicable to other 2D magnets as well

Sivadas, Okamoto, Xu, Fennie, DX Nano Lett. **18**, 7658 (2018);
Jiang et al PRB (2019); Soriano et al, Solid State Commun. (2019); Wang et al. Nat. Comm (2018)

Experimental evidence: SHG

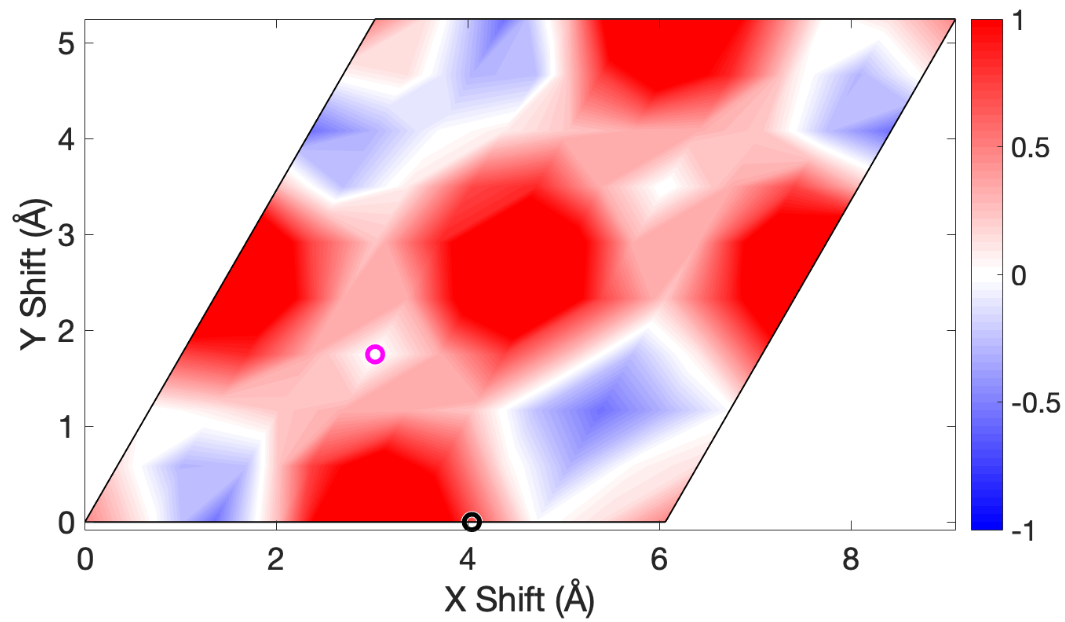


SHG angle dependence shows clear C_2 symmetry, consistent with monoclinic stacking (rhombohedral stacking should show C_3)

Sun, … DX, Wu, Xu, Nature (2019)

Stacking dependence in $CrCl_3$

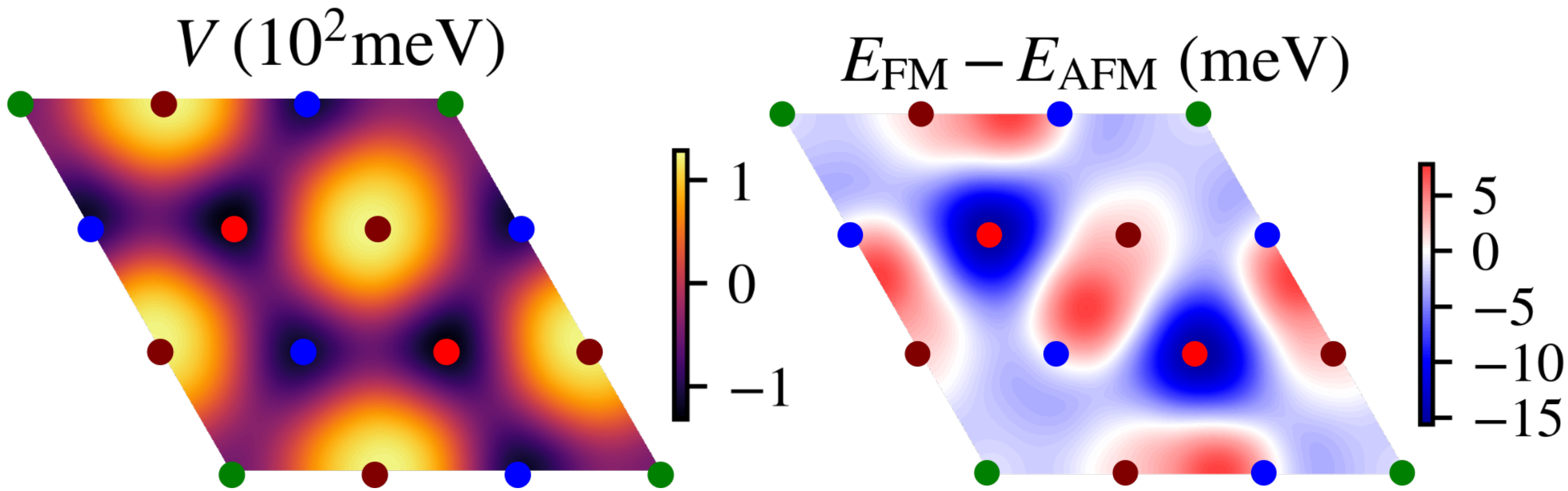
Similar map of interlayer exchange has been found in $CrCl_3$

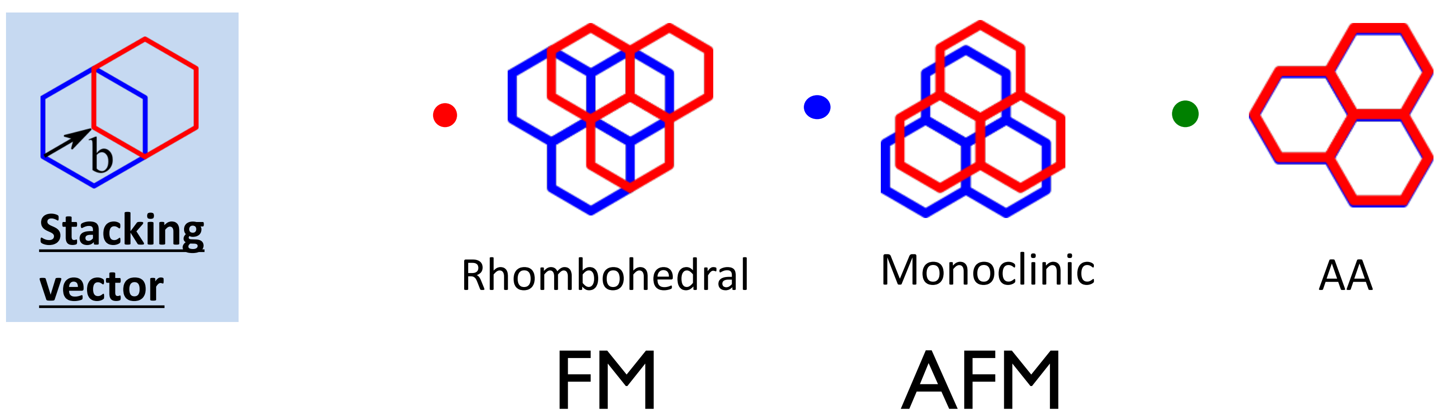


Klein et al, Nat. Phys. (2019)

What is the consequence of
stacking-dependent magnetism?

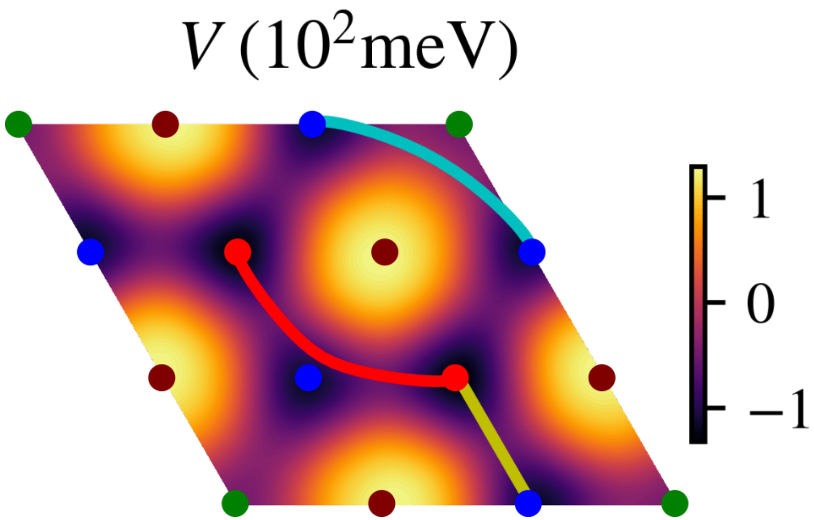
Stacking dependent magnetism





The interlayer binding energy is much larger than the exchange interaction.

Structural domain walls



Rhombohedral-Rhombohedral (RR)

Monoclinic-Monoclinic (MM)

Rhombohedral-Monoclinic (RM)

Energy of the domain wall

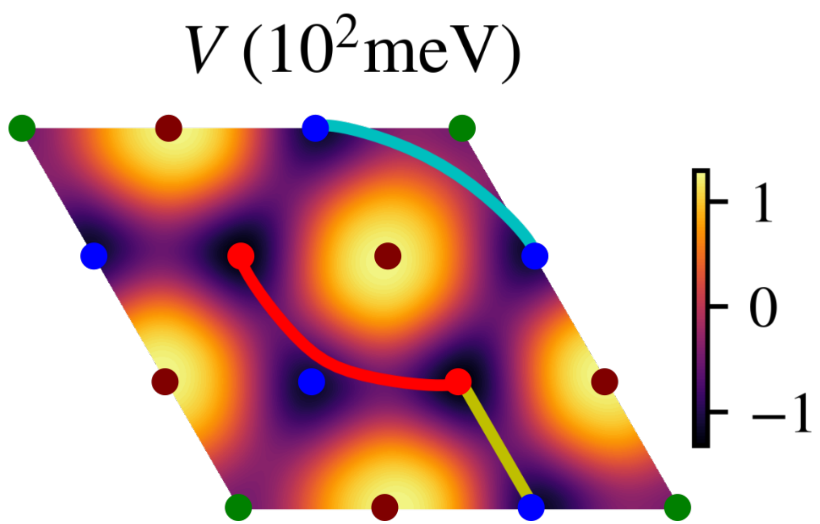
$$E_{\mathrm{str}} = \int \left[V(\boldsymbol{b}) + \frac{B+G}{4}(\partial_x b^x)^2 + \frac{G}{4}(\partial_x b^z)^2 \right] \mathrm{d}x$$

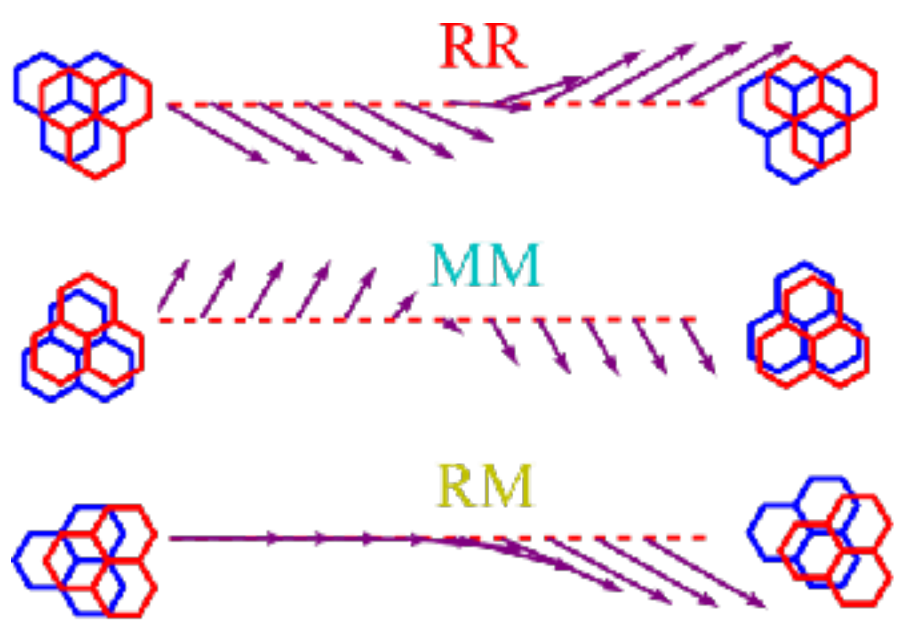
B= 54.307 eV and G = 39.248 eV are bulk and shear modulus (DFT)

Structural domain walls

Minimization is performed by solving the following differential equation:

$$\frac{\partial \boldsymbol{b}}{\partial t} = -\frac{\delta E_{\mathrm{str}}}{\delta \boldsymbol{b}}$$

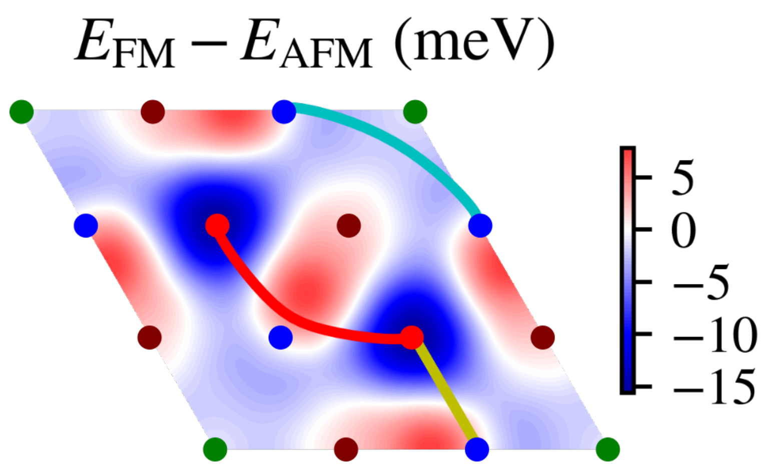


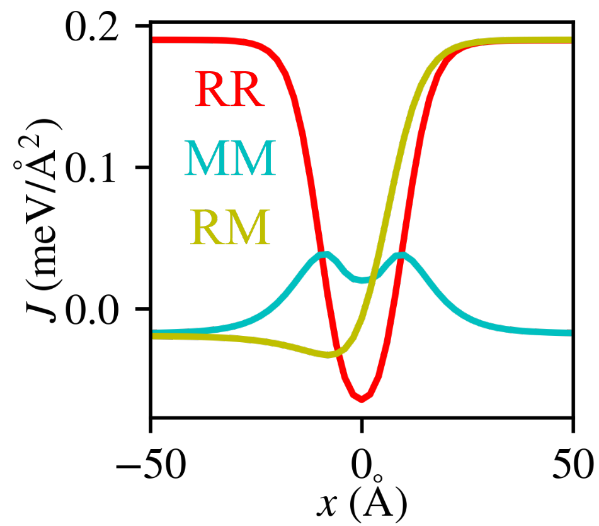


The RM domain wall can be described by the sine-Gordon equation

$$b^z = 2(b^z_{\mathrm{right}} - b^z_{\mathrm{left}})\arctan[\exp(x/w)]/\pi + b^z_{\mathrm{left}}$$

Variation of interlayer exchange

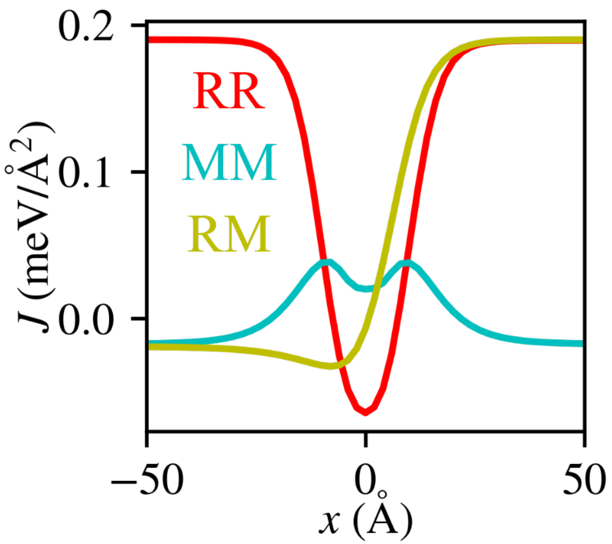




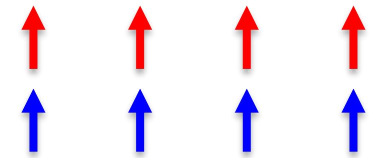
$$E_{\rm mag} = \int \left[\sum_{\alpha,\beta,l} \frac{A}{2} (\partial_\beta m_l^\alpha)^2 - \sum_l \frac{K}{2} (m_l^y)^2 - \sum_\alpha J m_1^\alpha m_2^\alpha \right] \mathrm{d}x$$

There are two magnon branches (The Cr atoms form a honeycomb structure.). We are only looking at the low-energy long wave-length limit.

Spin configuration of RR DW



R/R (FM/FM)



$$E_{\rm mag} = \int \left[\sum_{\alpha,\beta,l} \frac{A}{2}(\partial_\beta m_l^\alpha)^2 - \sum_l \frac{K}{2}(m_l^y)^2 - \sum_\alpha J m_1^\alpha m_2^\alpha \right] \mathrm{d}x$$

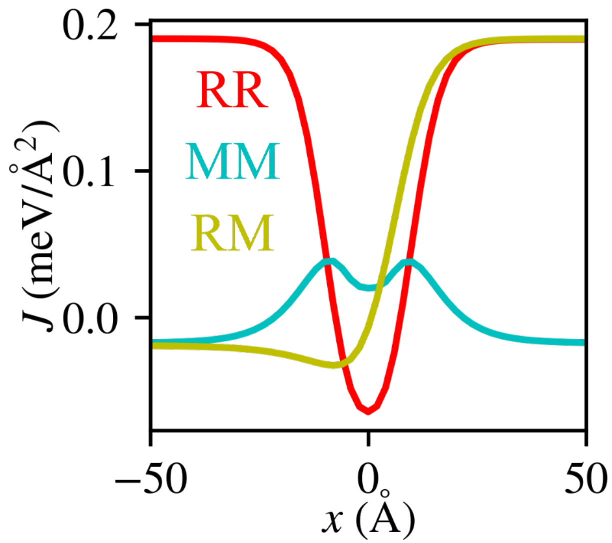
- Intralayer exchange prefers uniform spin configuration
- Easy-axis anisotropy also disfavors any spin rotation
- Inside the structural domain wall, interlayer exchange flips sign, which favors spin rotation

Magnetic structure of RR domain wall is uniform FM in the out-of-plane direction

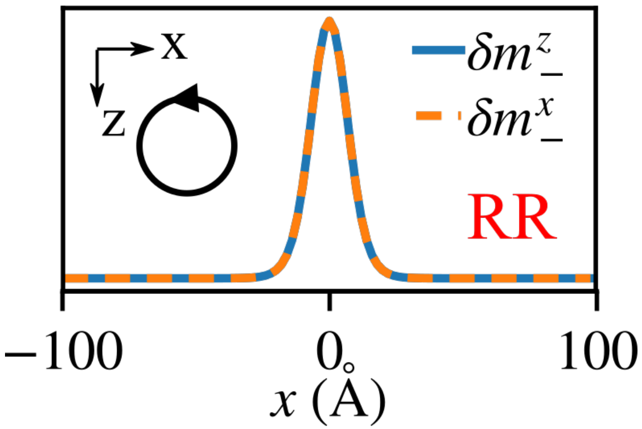
Spin dynamics of RR DW

$$\delta \boldsymbol{m}_{\pm} = \delta \boldsymbol{m}_1 \pm \delta \boldsymbol{m}_2$$
$$\delta m_{\pm}^{+} = \delta m_{\pm}^{x} + \mathrm{i}\delta m_{\pm}^{z}$$

$$\mathrm{i}\gamma^{-1}\partial_t \delta m_{+}^{+} = [-A\nabla^2 + K]\delta m_{+}^{+}$$
$$\mathrm{i}\gamma^{-1}\partial_t \delta m_{-}^{+} = [-A\nabla^2 + K + 2J(x)]\delta m_{-}^{+}$$



- δm_+ is blind to interlayer exchange coupling J(x)
- J(x) acts like a trapping potential for δm_-

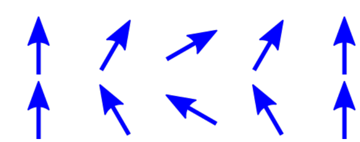


δm_- is a trapped magnon mode (~ 0.3 K = 0.09 meV)

Universal existence of DW magnons

$$i\gamma^{-1}\partial_t \delta m_-^+ = [-A\partial_x^2 + K + 2J(x) + Ak_z^2]\delta m_-^+$$

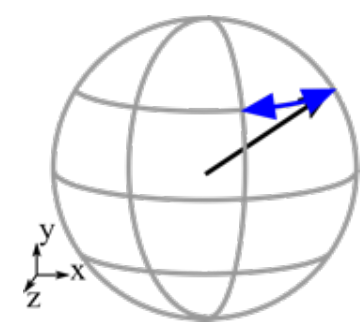
- Beyond a critical point, the magnetic ground state deviates from interlayer FM



- The magnetic energy

$$E_{\mathrm{mag}} = \int \left[\sum_{\alpha,\beta,l} \frac{A}{2}(\partial_\beta m_l^\alpha)^2 - \sum_l \frac{K}{2}(m_l^y)^2 - \sum_\alpha J m_1^\alpha m_2^\alpha \right] \mathrm{d}x$$

respects continuous rotational symmetry in the out-of-plane direction

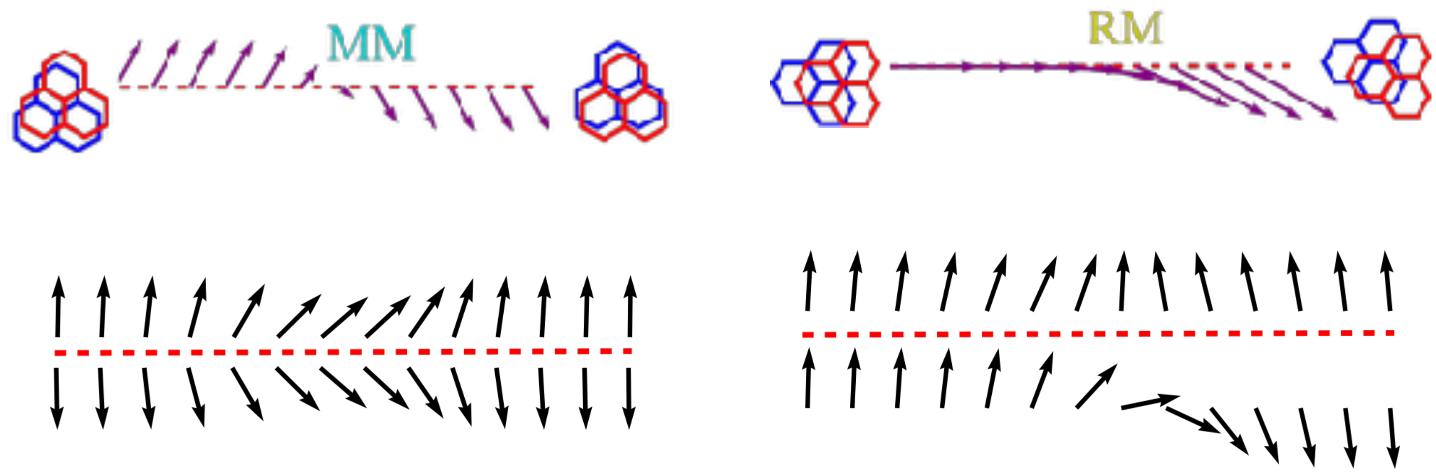


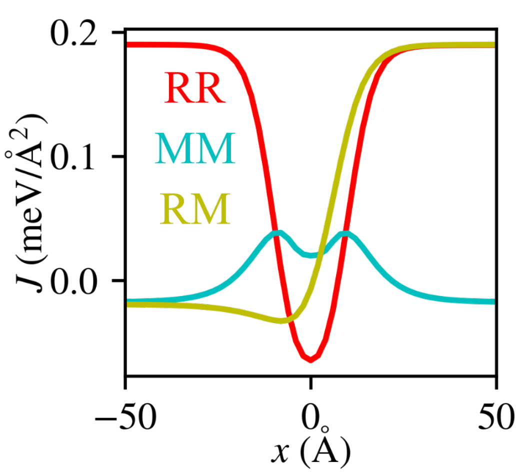
- Goldstone magnon mode exists in the DW

MM and RM domain walls

Stacking Vector

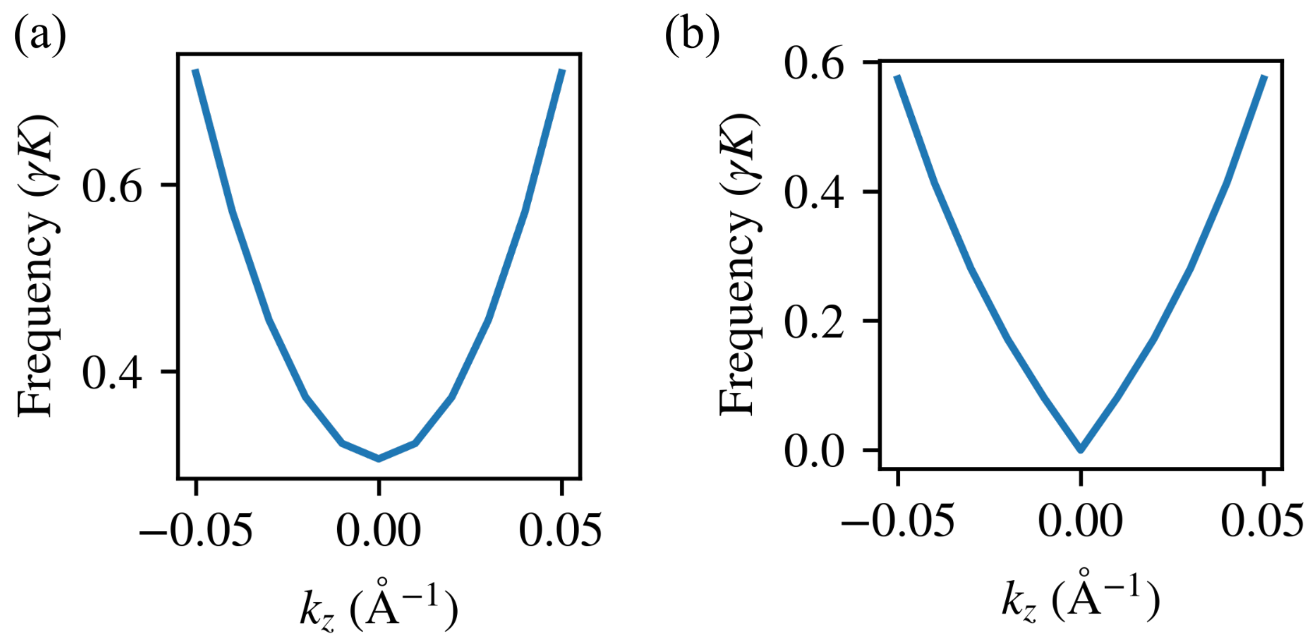
Spin Config.





- Both domain walls support Goldstone modes.
- Numerically verified by solving the LLG equation

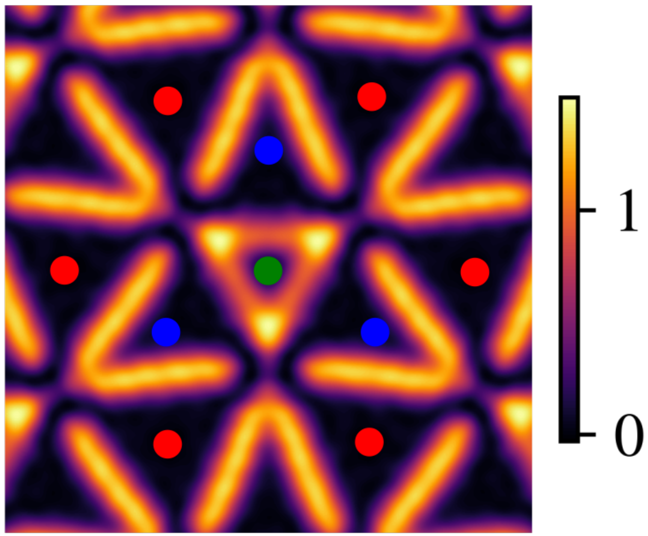
Magnon disperson



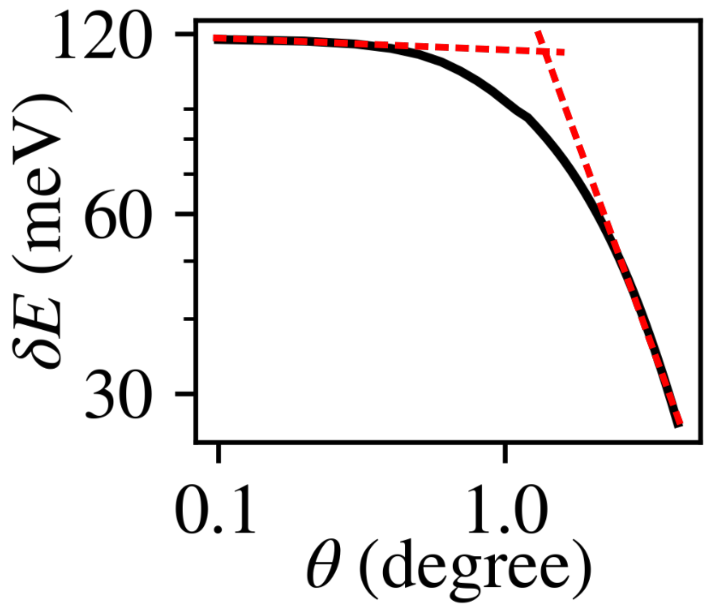
R/R(FM/FM)

M/M(AFM/AFM)

Twisted bilayer CrI_3

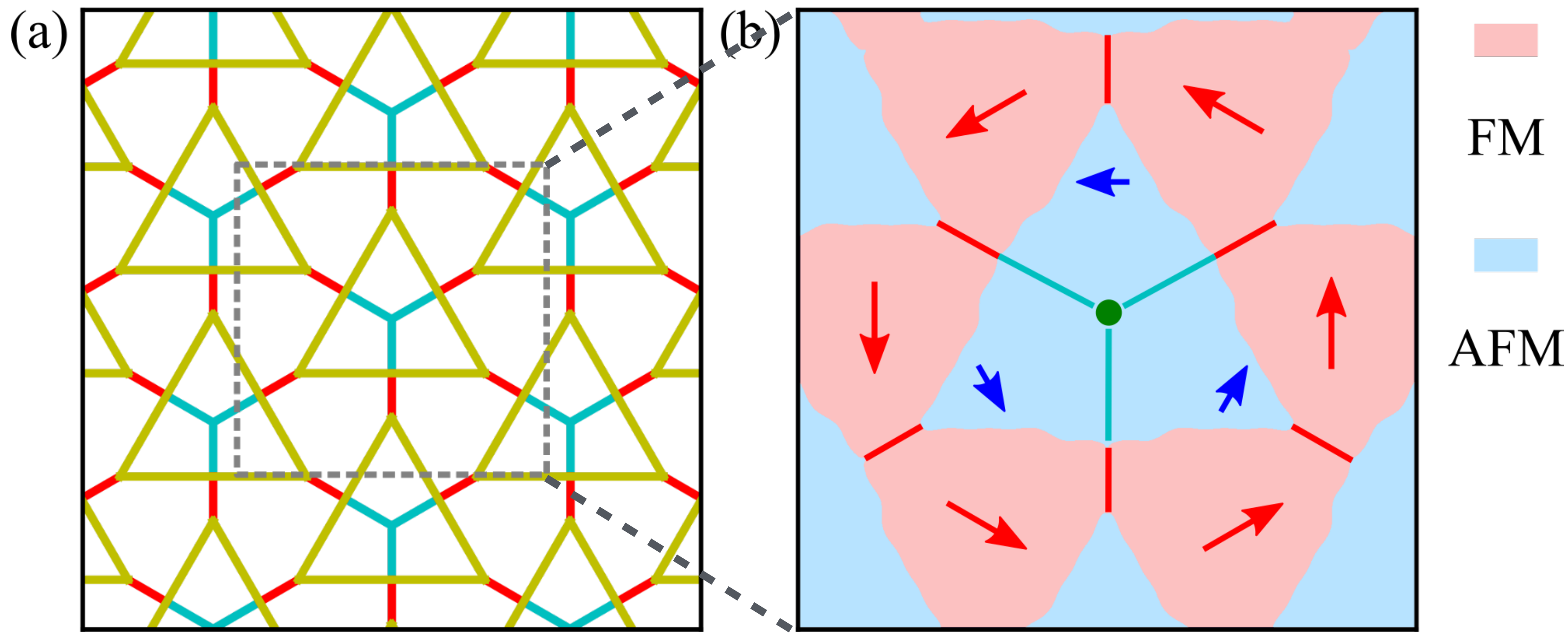


Shear strain at 2 degree



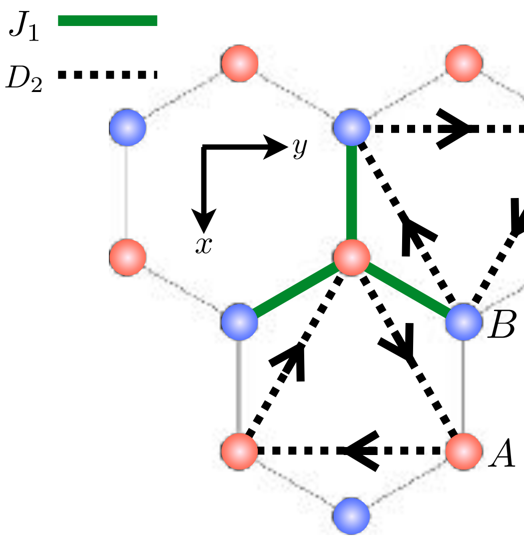
- At large twisting angle, a metastable domain (green dot) appear
- Lattice relaxation has a sudden onset as a function of twisting angle (~ 1 degree)

Moire Magnon network

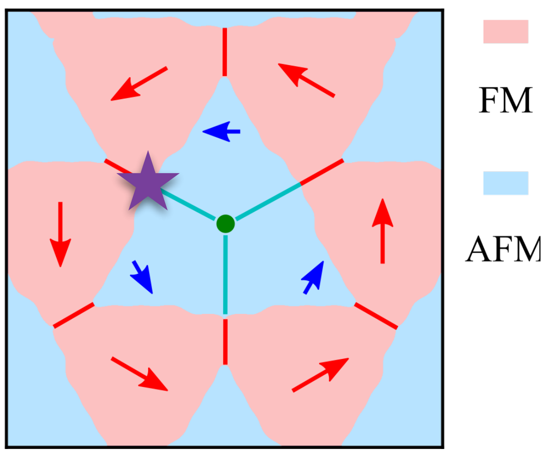


- Moire magnon network at 0.1 degree.
- There are trapped magnon modes on the FM/FM and AFM/AFM domain walls

Discussion



In general, honeycomb lattice allows a 2nd order DMI [Owerre, JAP 2016, Kim et al, PRL 2016, Cheng, Okamoto, DX PRL 2016], which realize a magnonic version of the Haldane model for honeycomb FM. The topological edge mode is about 15 meV



We essentially deal with 1D solitons. What happens at the corners where the magnon modes merge? [Hejazi, Luo and Balents, PNAS 2020]

Summary

- All stacking domain walls of bilayer CrI_3 support 1D trapped magnons. Since stacking domain walls are insensitive to external fields, these magnon modes can serve as robust 1D information channels.
- Small angle twist bilayer CrI_3 hosts a 1D magnon network.
- Stacking domain walls are important in understanding magnetic properties of van der Waals magnets, and offer new way of stacking engineering of magnetic dynamics.

arXiv:2007.10398