A55.007: Room 305, Mon. March 6

# Skyrmions in van der Waals centrosymmetric materials

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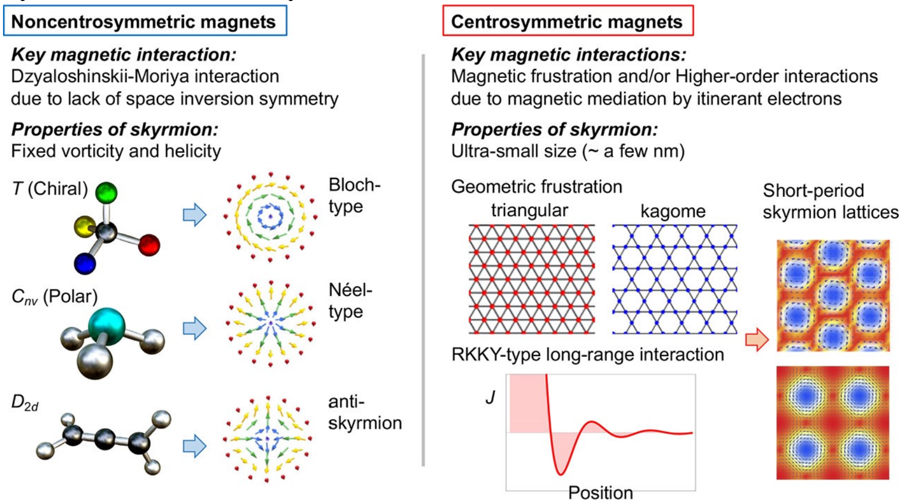
# Introduction

## Noncentrosymmetric vs Centrosymmetric




**Searching new mechanism to stabilize skyrmions in centrosymmetric lattice is urgent task**

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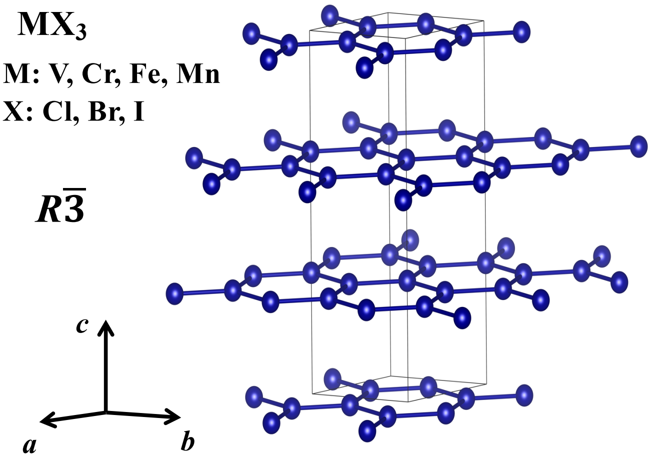
## Introduction
## Target materials

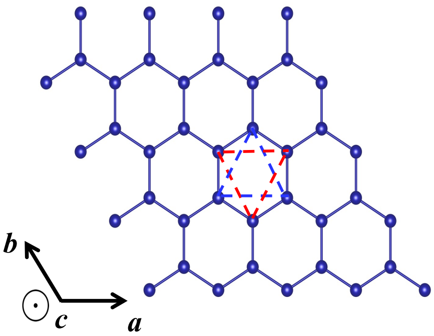
**$MX_3$**

**M: V, Cr, Fe, Mn**

**X: Cl, Br, I**

$R\bar{3}$




Dzyaloshinskii-Moriya interactions of 2nd NN can be finite

**Purpose:** To investigate the effect of Dzyaloshinskii-Moriya interactions on magnetic properties of van der Waals centrosymmetric $MX_3$

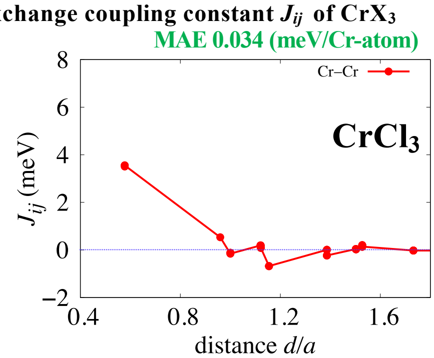
## Methods

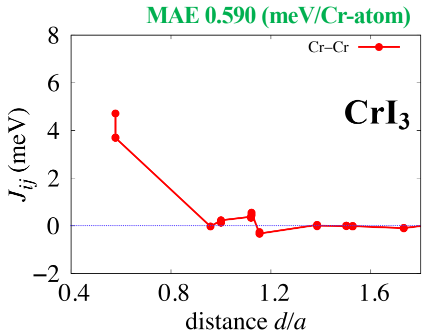
### Classical Heisenberg model with Dzyaloshinski-Moriya interaction

$$H_{\mathrm{Heis}} = \underbrace{-\sum_{<ij>} J_{ij}^{m}\vec{S_i}\cdot\vec{S_j}}_{\text{Isotropic exchange}} \underbrace{-\sum_{<ij>} \vec{D_{ij}}\cdot(\vec{S_i}\times\vec{S_j})}_{\text{Antisymmetric exchange}} \underbrace{-\sum_{i} k_{\mathrm{u}}(\vec{e_u}\cdot\vec{S_i})^2}_{\text{Uniaxial anisotropy}} \underbrace{-g\mu_{\mathrm{B}}\sum_{i}\vec{H_{\mathrm{ext}}}\cdot\vec{S_i}}_{\text{Zeeman}}$$

## Results and Discussions

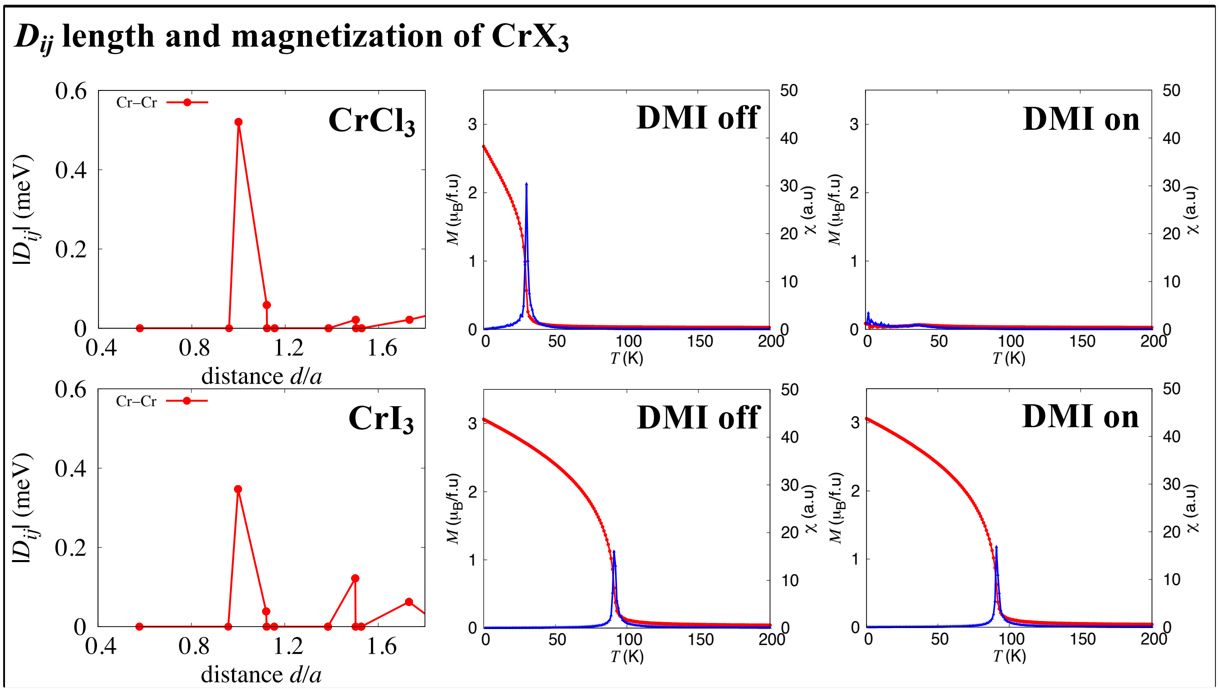
**Isotropic exchange coupling constant $J_{ij}$ of $CrX_3$**




We use classical Heissenberg model with isotropic exchange, antisymmetric exchange or DMI, uniaxial anisotropy, and Zeeman term. All parameters of Monte Carlo simulations are obtained from first principles calculations.

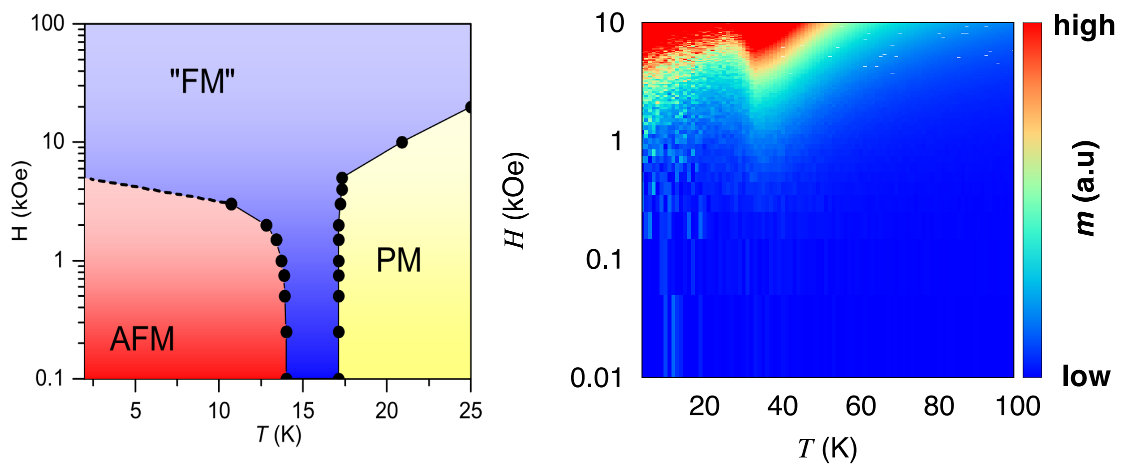
First we consider the magnetic exchange coupling constants Jij in CrX3. When X change from Cl to I, the magnetocrystalline anisotropy increase from 0.034 to 0.590 meV/ Cr-atom. The positive value of MAE mean the easy axis is out of plane, the c direction. In additions, the interlayer exchange coupling constant in CrCl3 is positive. So it does not support the in plane AFM in experimental paper.




Then we consider the DMI in first principles calculations. The DMI of second nerest neighbor of intralayer is finite and quite large even in CrCl3. As point out in previous slide, the results of MAE and Jij in CrCl3 does not suport the inplane AFM in experimental works. And if we calculated the magnetization with switch off DMI, all CrX3 shows clear FM-PM transition with the ground state being FM.

But if we include the DMI in simulations, the FM in CrCl3 is disappeared while the FM-PM transition is maintained in CrBr3 and CrI3 due to high MAE. So with the DMI in simulation, we can get zero magnetization and magnetic susceptibility in CrCl3, similar behavior with experimental of inplane AFM order.

**Comparison of magnetic phase diagram of $CrCl_3$**

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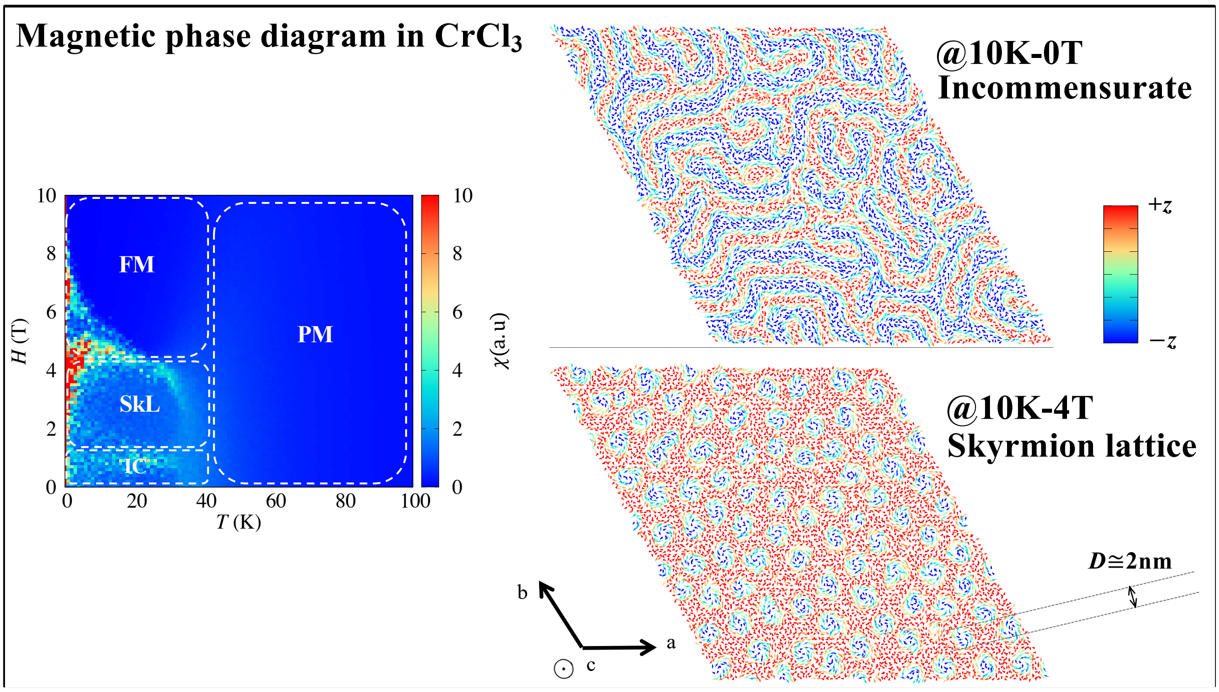
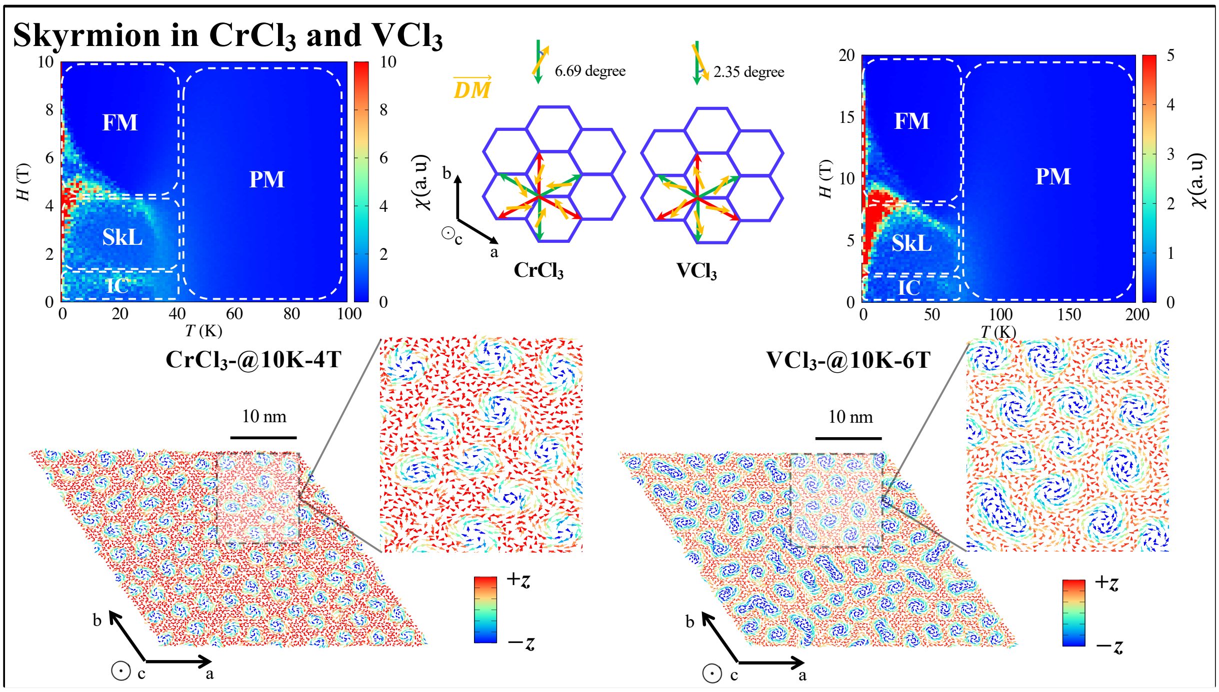
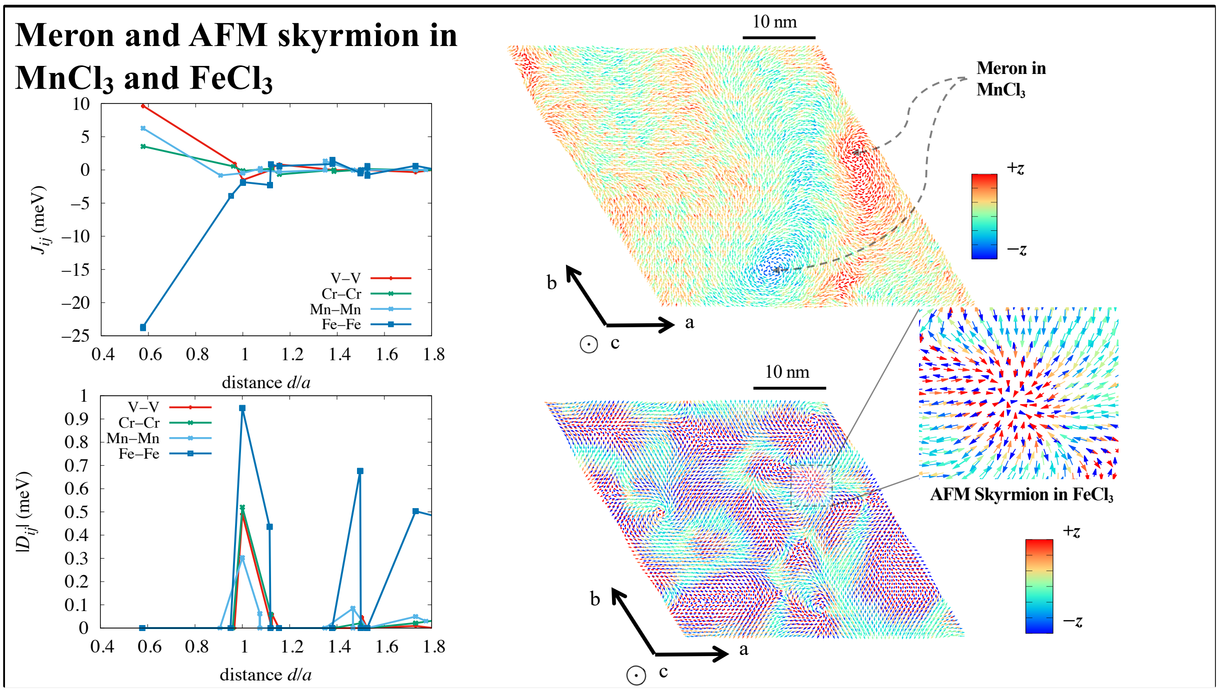
Then we calculate the magnetic phase diagram of CrCl3. the blue color means magnetization is small, it is AFM or PM in experimental phase diagram. The red color means the magnetization is high, it is FM in experimental. Here at this temperature, the red region is expand in low magnetic field region. We got a good agreement with experimetal study.




Then we check the snapshot of Monte Carlo simulations for making the magnetic phase diagram in magnetic susceptibility. At 10 K and 0 T, the magnetic phase is incomensurate with broken of long range order. If we apply magnetic field like 4 T, we can get the skyrmion lattice in CrCl3.




We also found that VCl3 also have similar magnetic phase diagram as CrCl3. However, the DM vector of VCl3 is nearly opposite with CrCl3. It leads to two type of skyrmion with diferent helicity. If we can control the electron or hole dope in multilayer, we might control the helicity of the materials. Note that the skyrmion diameter is quite small, about 2 nm due to the centrosymmetric materials.




We also found the Meron in MnCl3 and AFM skyrmion in FeCl3. In MnCl3, the magnetic anisotropy is easy plane with ab plane, it leads to the formation of Meron at zero external magnetic field.

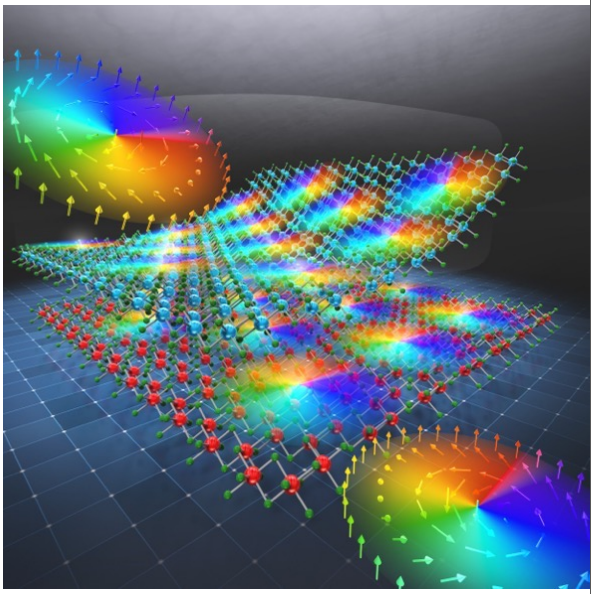
In FeCl3, the magnetic exchange coupling constants is negative, so it prefer AFM order. The AFM skyrmion has advantage that the hall velocity is approximately equal to zero, so it can survivor for long time.

## Summary

New mechanism to stabilize skyrmions in van der Waals centrosymmetric material

Not only skyrmions but also meron and antiferromagnetic skyrmions are observed

$VCl_3$ and $CrCl_3$ shows posibility to control helicity by heterostructure and electric field



H. B. Tran, Y. Matsushita, arXiv:2209.02333(2022)

**Thank you so much for kind attentions!**

That all for our talk today, thank you so much for kind attentions.