



Bloch-type



Neel-type



Theoretical Study of Skyrmions in Two-dimensional Materials

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Advisor: Prof. Yandong Ma

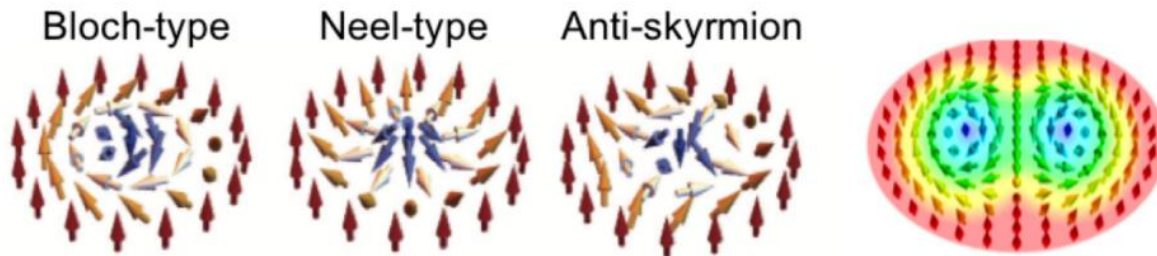
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$$Q = \frac{1}{4\pi} \int_S \mathbf{n}(\mathbf{r}) \cdot [\partial_i \mathbf{n}(\mathbf{r}) \times \partial_j \mathbf{n}(\mathbf{r})] d\mathbf{r}$$

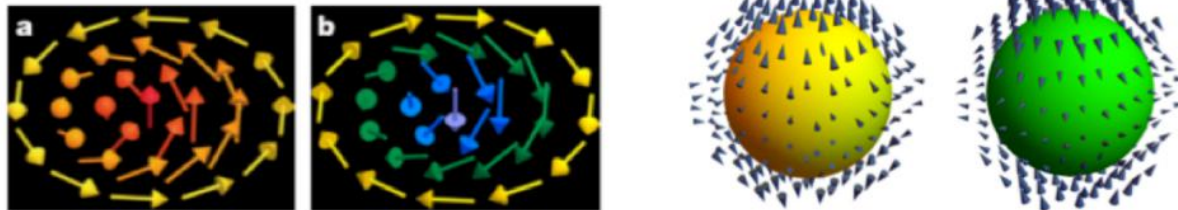
a Skyrmions ($Q = \pm 1$)

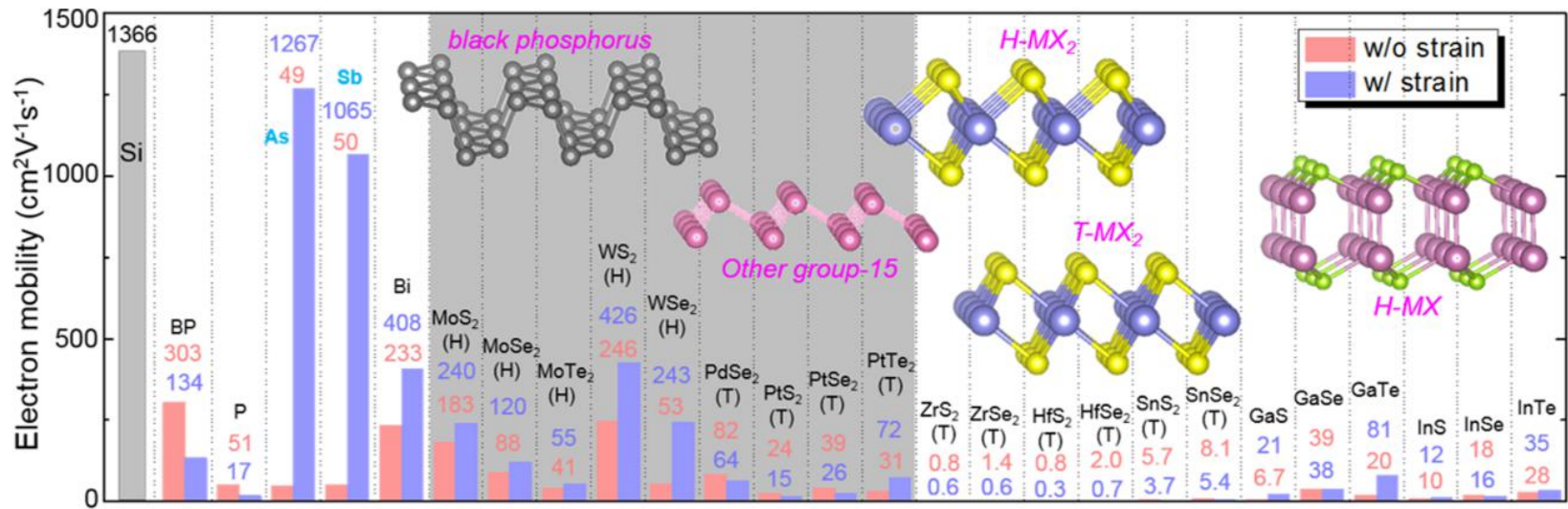
b Biskyrmion ($Q = -2$)



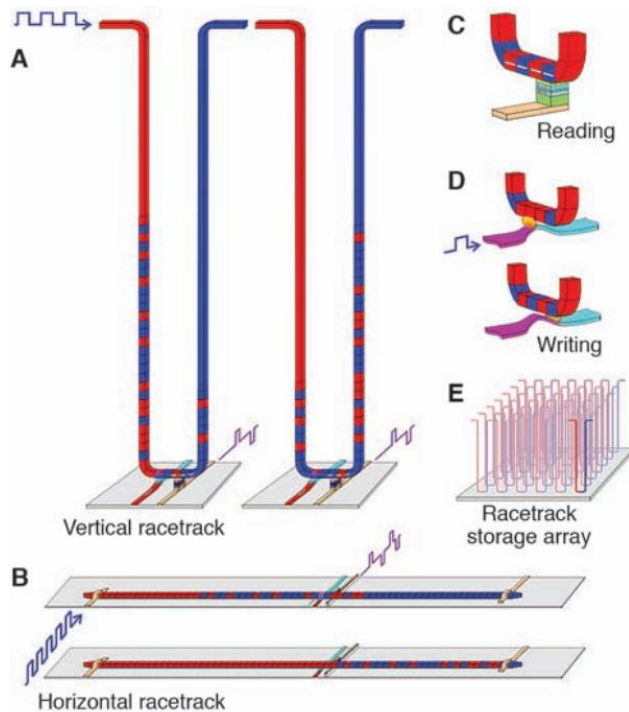
c Merons ($Q = \pm 1/2$)

d Hedgehogs ($Q = \pm 1$)

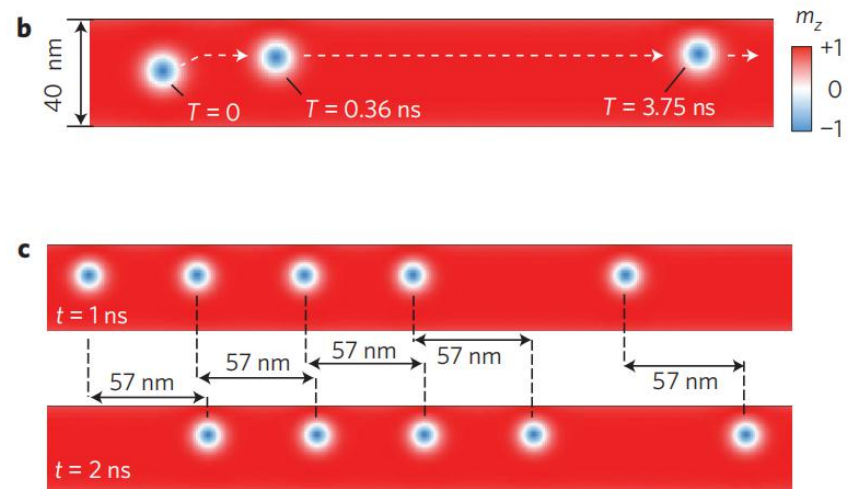




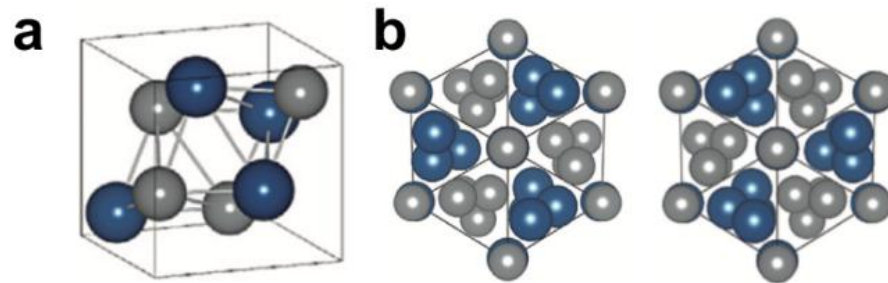
Y. Liu*, PRL.125,177701 (2020)



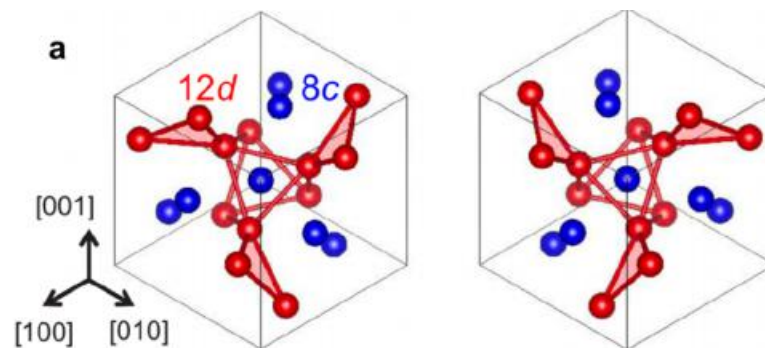
S. S. P. Parkin*, Science 320,5873 (2008)



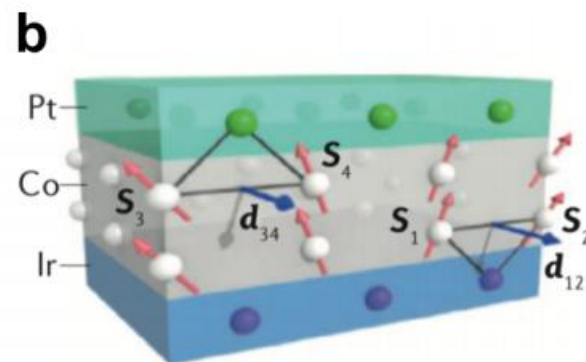
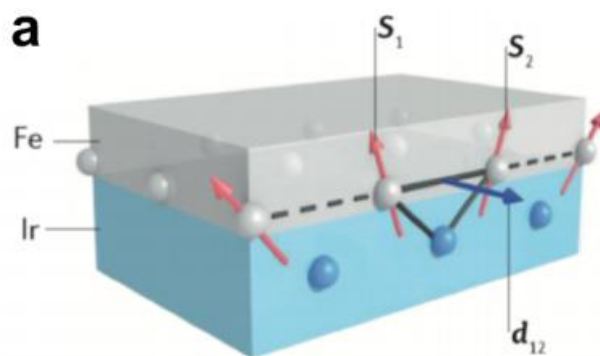
V.Cros*, Nat. Nanotech. 8, 839–844 (2013)



Science 323, 915–919 (2009)



PRB. 98, 155120 (2018)



Nat. Rev. Mater. 2, 17031 (2017)

How to Make Skyrmions Be Born in Monolayers?

Heisenberg exchange interaction

$$H_{EX} = -J [S_i \cdot S_j]$$

Dzyaloshinskii-Moriya interaction

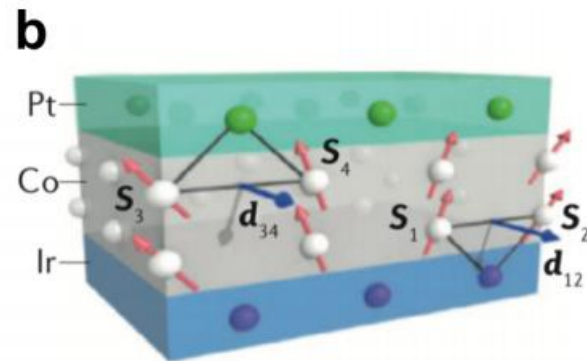
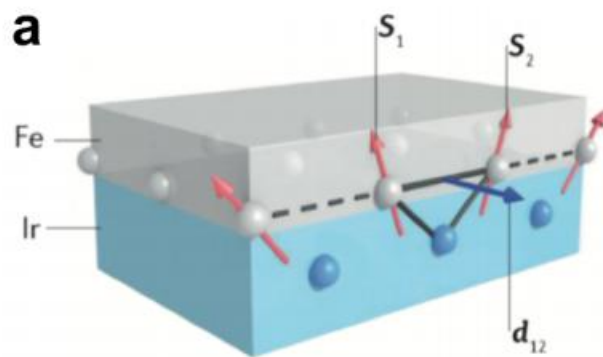
$$H_{DM} = D \cdot [S_i \times S_j]$$

Spin-Orbital Coupling

Heisenberg VS DMI

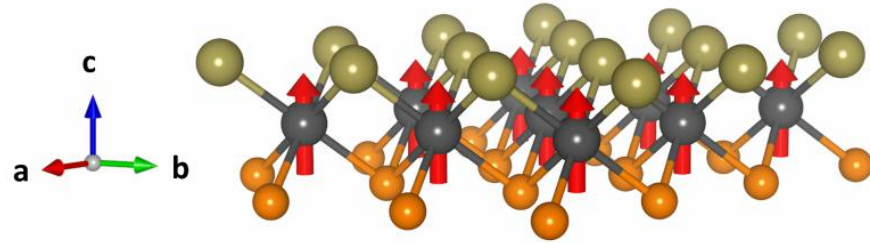


Inversion Symmetry Broken

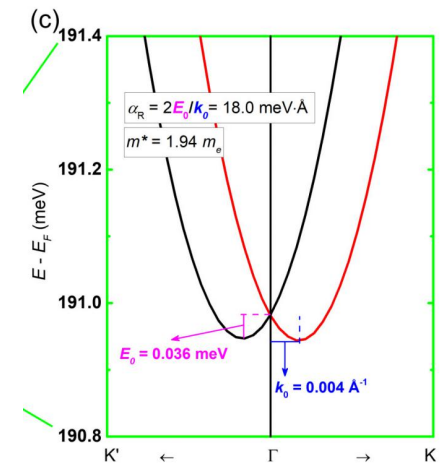
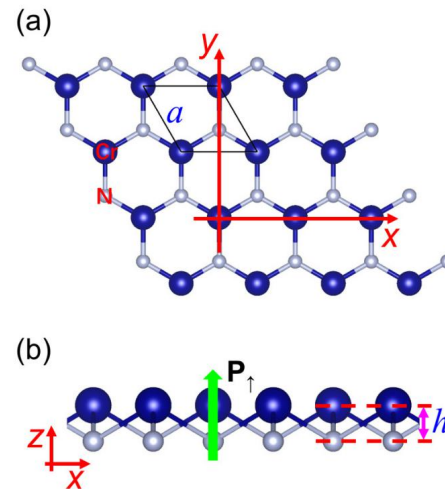


Monolayer with Inversion Symmetry Broken

Janus Monolayers



Monolayers with Rashba Effect



Computational Method

$$H = - \sum_{\langle i,j \rangle} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) - J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \lambda \sum_{\langle i,j \rangle} S_i^z S_j^z - K \sum_i (S_i^z)^2 - \mu_{Mn} B \sum_i S_i^z$$

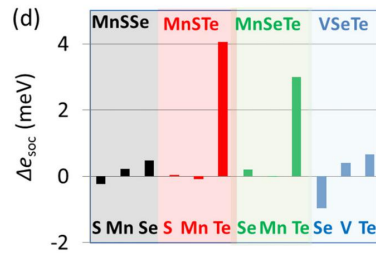
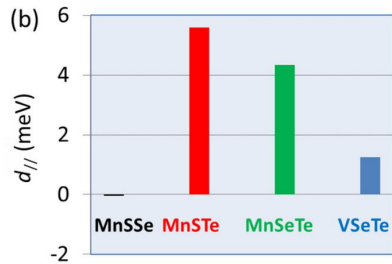
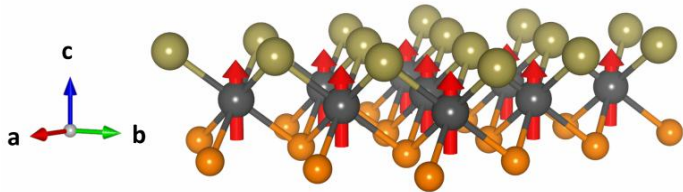
DFT + GPU-accelerated Monte Carlo



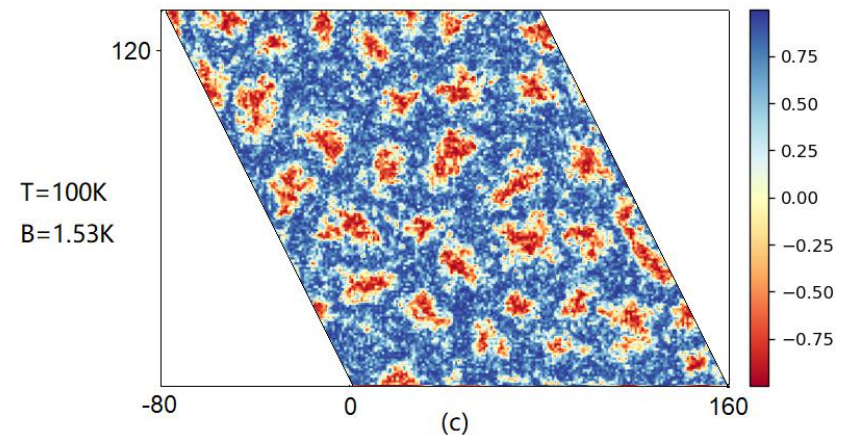
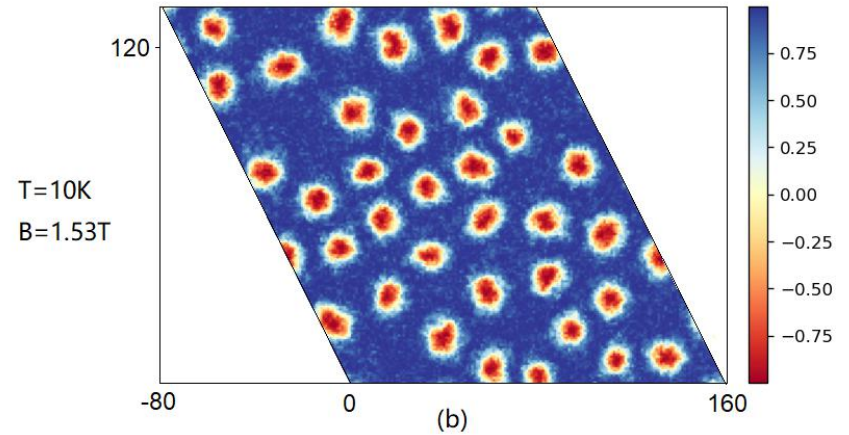
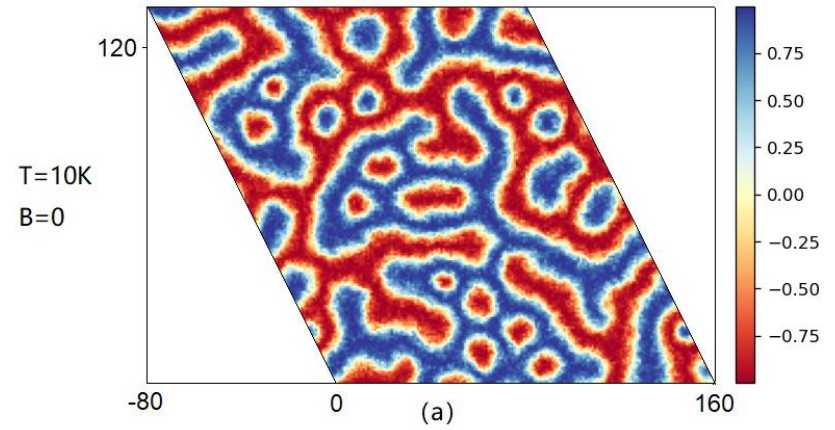
+



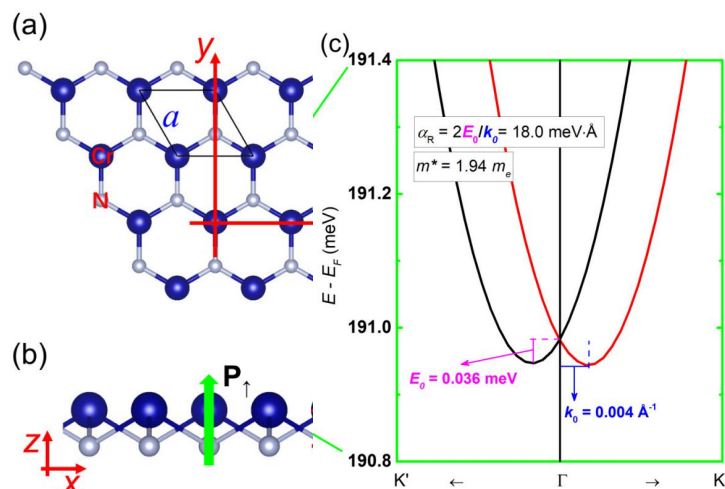
Janus Monolayers



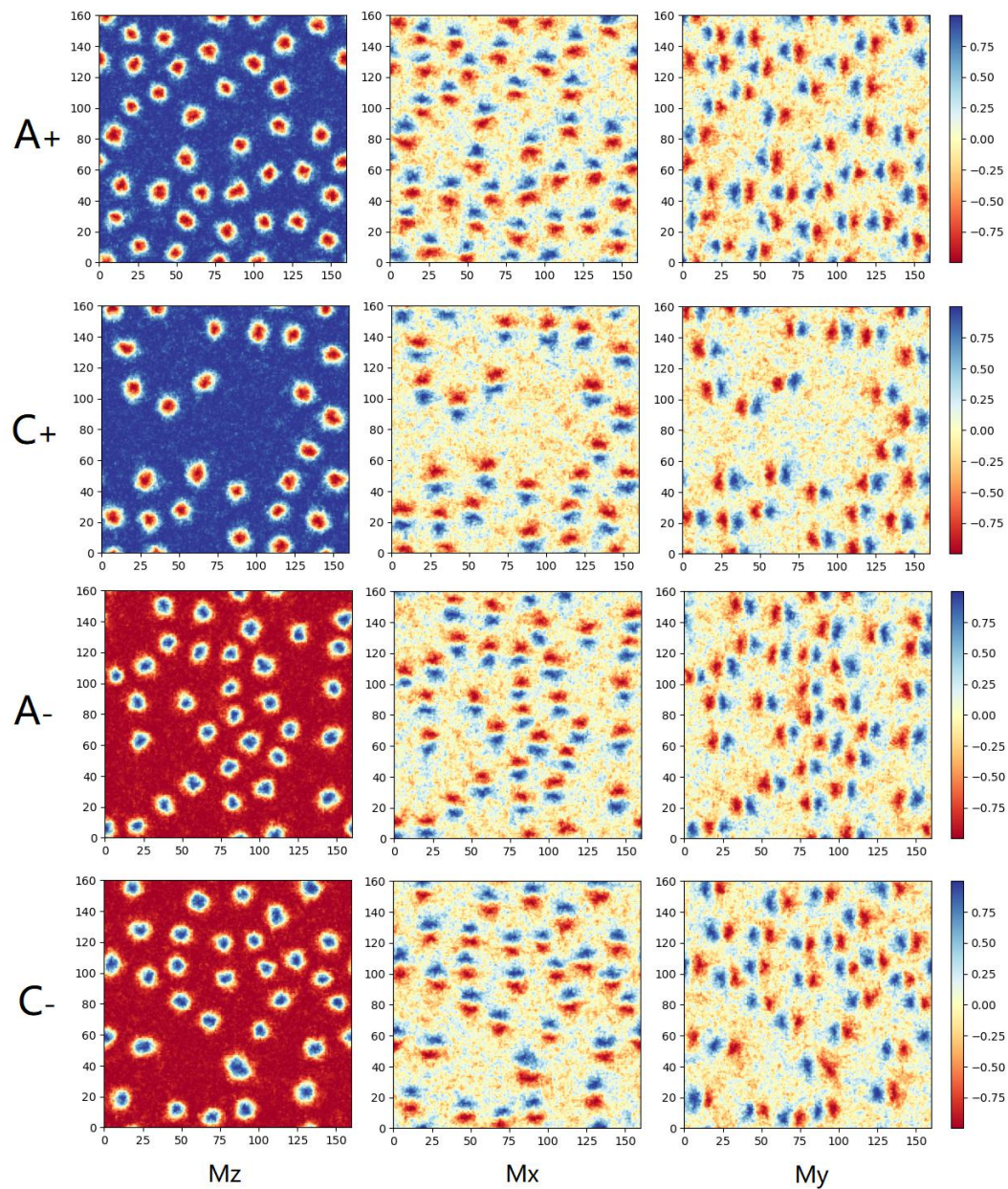
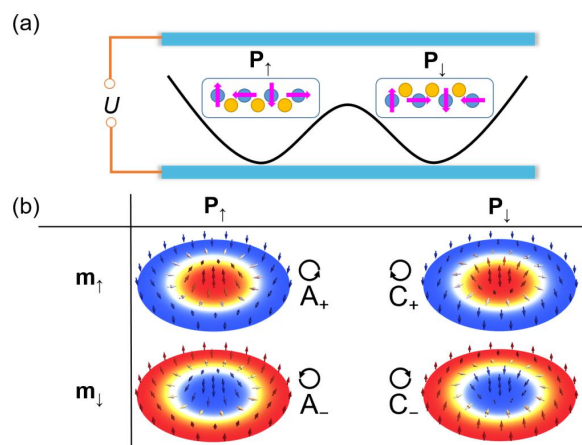
Fert-levy Mechanism



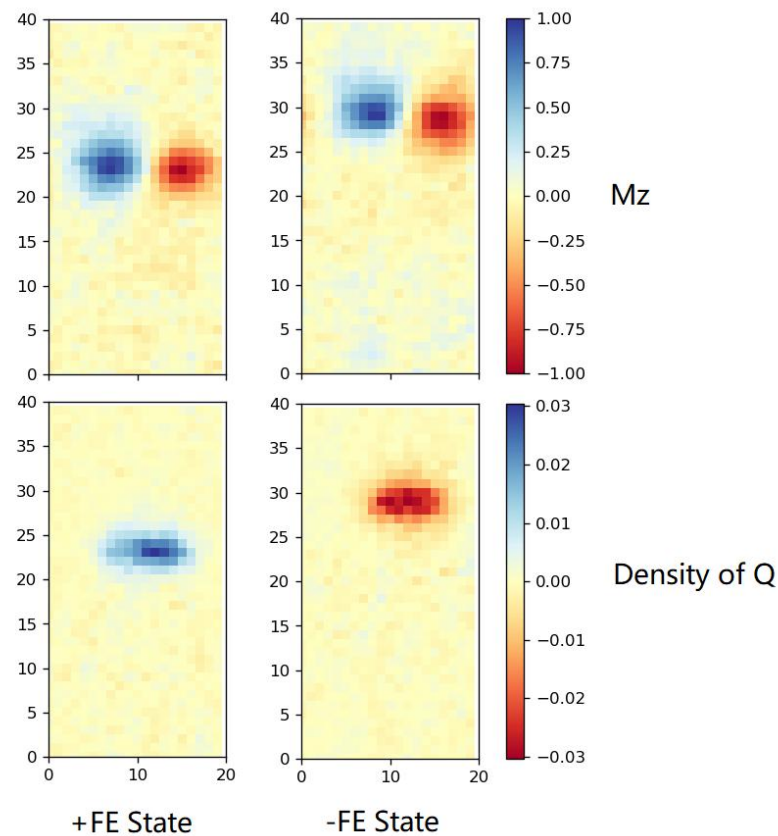
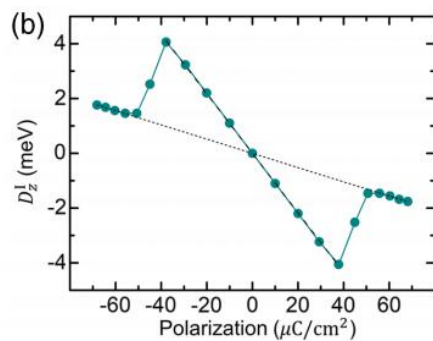
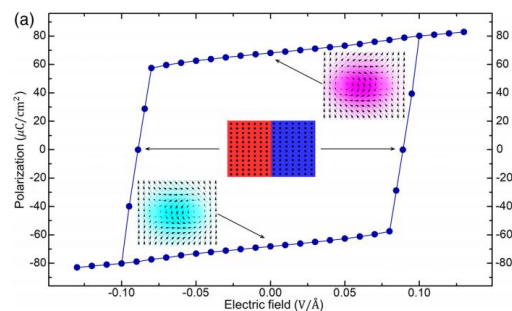
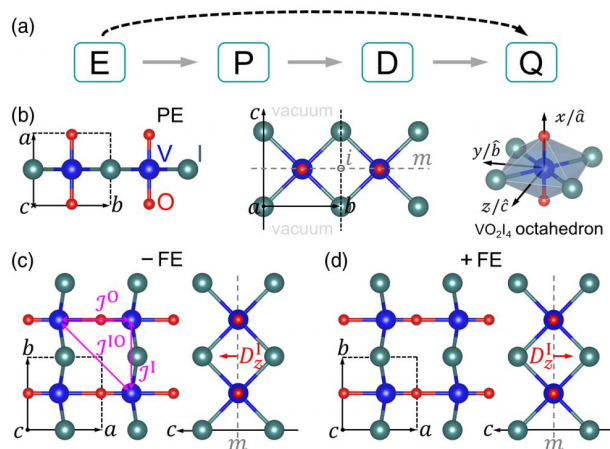
Monolayers with Rashba Effect



Rashba-induced DMI



Topological Phase Transition



Bloch-type



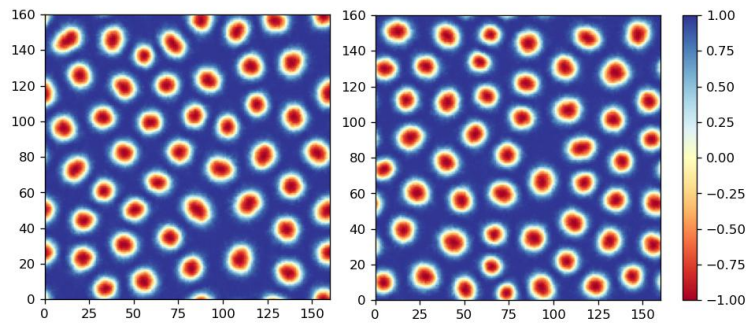
Neel-type



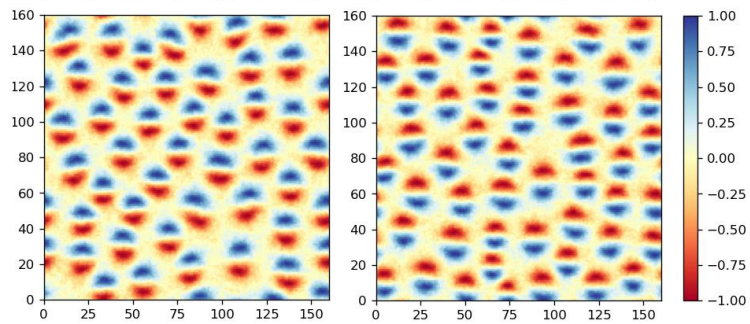
Anti-skyrmion



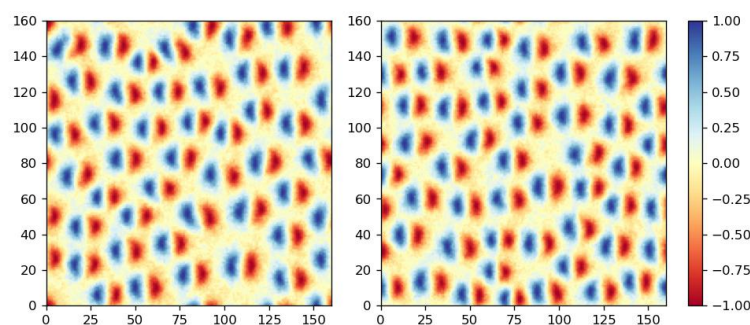
Anisotropic DMI with opposite signs along two orthogonal in-plane directions?



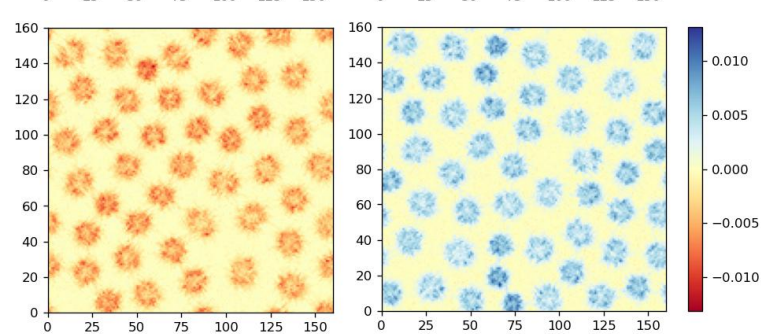
M_z



M_x



M_y



Density
of Q

$Dx=3.0\text{meV}$
 $Dy=3.0\text{meV}$

$Dx=3.0\text{meV}$
 $Dy=-3.0\text{meV}$



skyrmion

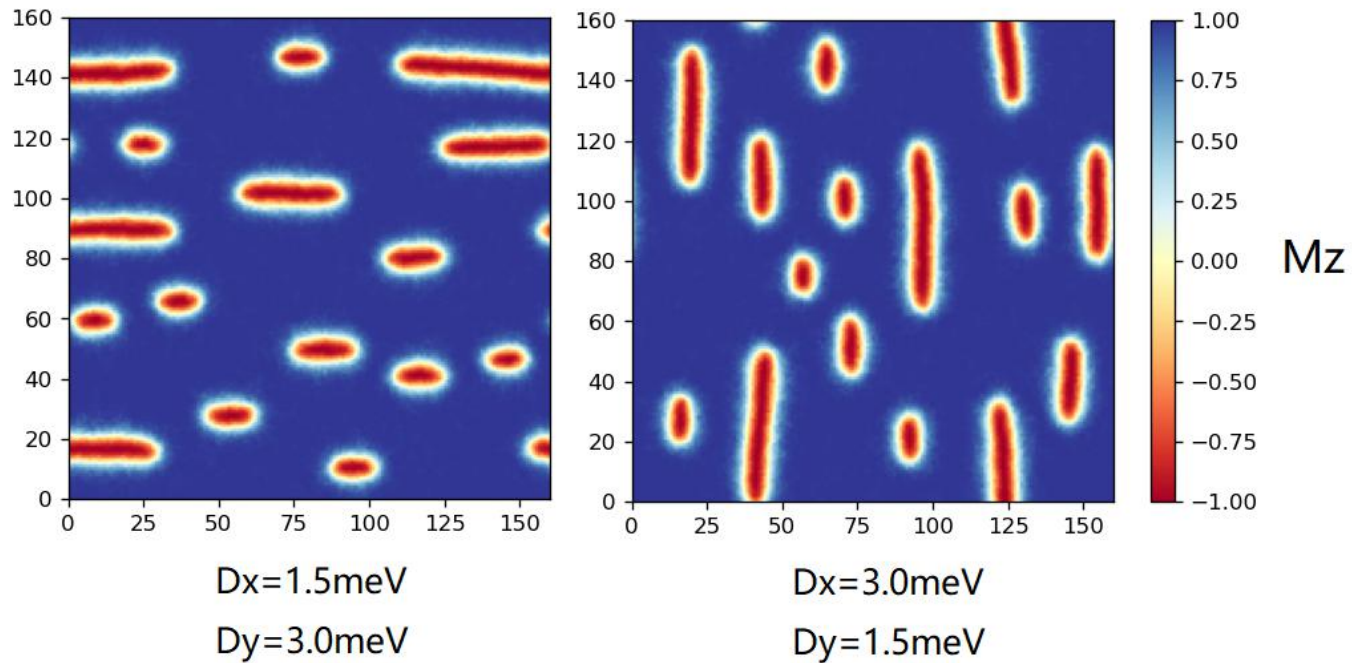


EPDQ



antiskyrmion

Anisotropic DMI



Generating new degree of freedom

Eliminating skyrmion Hall effect

Prospectives

Stablizing skyrmions in monolayers

**Forming topological phase transitions in 2D
multiferroic materials**

Anisotropic DMI controlled by external fields

Thanks